Electronic Supplementary Material (ESI) for Green Chemistry.

Iron(II)-catalyzed intermolecular aziridination of alkenes employing hydroxylamine derivatives as clean nitrene sources

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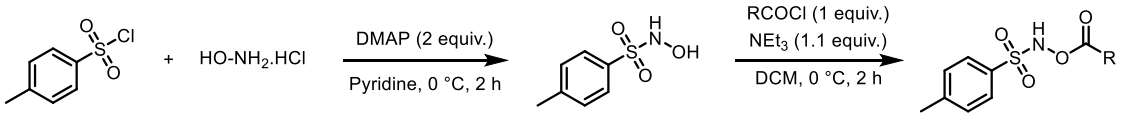
I. General Information

All commercially available reagents were purchased from chemical suppliers. Styrene derivatives were used without further purification; alkyl alkenes were distilled just before using. Reactions were performed under an argon atmosphere. Anhydrous solvents were purchased from chemical suppliers and used without further purification. Analytical thin layer chromatography was performed on commercial silica gel plates $60F_{254}$. Flash column chromatography was performed on silica gel 60 (40−63 μm). NMR spectra were recorded on a 500 MHz spectrometer. Chemical shifts (δ) are reported in ppm relative to tetramethylsilane (δ 0.00 ppm) or the $CHCl_3$ residual peak (δ 7.26) or the MeOH residual peak (δ 3.31) for ^{1}H NMR. Chemical shifts of ^{13}C NMR are reported relative to $CDCl_3$ (δ 77.16) or CD_3OD (δ 49.00). Coupling constant (*J*) are reported in Hertz unit (Hz). Multiplicities are described with standard following abbreviations: s = singlet, br = broad, d = doublet, t = triplet, q = quadruplet, dd = doublet of doublet, dt = doublet of triplet, m = multiplet. High resolution mass spectra (HRMS) were recorded with a TOF mass analyzer under electrospray ionization (ESI) in positive or negative ionization mode detection, atmospheric pressure chemical ionization or atmospheric pressure photoionization (APPI). Melting points were measured on a Köfler bench. IR spectra were recorded on a FT-IR spectrophotometer, and the wavelengths reported in cm^{-1}.

II. Preparation of reagents and general procedures

Synthesis of hydroxylamine derivatives:



Preparation of *N*-tosyl hydroxylamine:

The *N*-tosyl hydroxylamine compound was prepared using a modified literature procedure.[1] Pyridine (5 mL) was added to the flask containing hydroxylamine hydrochloride (1.094 g, 15.74 mmol, 2 equiv.) at 0 °C. The solution was stirred until the hydroxylamine hydrochloride was mostly dissolved. DMAP (1.92 g, 15.74 mmol, 2 equiv.) was then added to the solution, and the suspension was stirred at 0 °C for 10 mn. Tosyl chloride (1.5 g, 7.87 mmol, 1 equiv.) was then added portion-wise whilst stirring, making sure to keep a flow of argon through the flask.

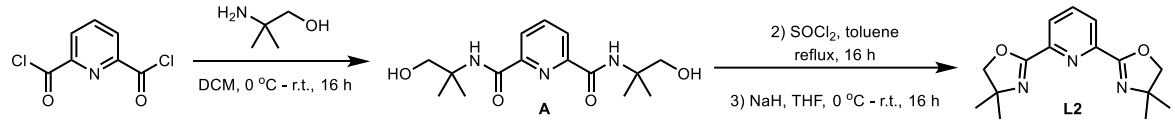
[1] K. Aizawa, H. Nakagawa, K. Matsuo, K. Kawai, N. Ieda, T. Suzuki and N. Miyata, *Bioorganic Med. Chem. Lett.*, 2013, **23**, 2340–2343.

The suspension was left to stir for 1-2 hours (reaction was followed by TLC) until full consumption of tosyl chloride. The reaction mixture was then quenched with an aqueous 1 M HCl solution (20 mL) and the aqueous phase was extracted with ethyl acetate. The organic phase was collected and washed twice more with 1 M HCl (20 mL) until the aqueous phase was pH 2-3. The combined acidic aqueous phases were extracted once more with ethyl acetate (20 mL). The combined organic phases were then dried over $MgSO_4$ and concentrated under reduced pressure forming a slightly yellow solid. The solid was washed with cold DCM to afford a white/slightly yellow solid (1.1 g, 75 %). Analytical data in accordance to the literature.[1]

General procedure for acylation of *N*-tosyl hydroxylamine:

To a solution of *N*-tosyl hydroxylamine (1 equiv.) in DCM (C = 0.2 M) under argon at 0 ^oC, triethylamine (1.1 equiv.) was added in one portion. The solution was stirred for 5 mn until all solids were dissolved. A solution of acyl chloride (1 equiv.) in DCM was slowly added dropwise to the solution containing the hydroxylamine at 0 ^oC. The reaction was left to stir for 1 h allowing the reaction to warm to room temperature. The mixture was then quenched with an aqueous saturated NH_4Cl solution and the aqueous phase was extracted with DCM (3 times). The organic phases were combined, dried over $MgSO_4$ and concentrated under reduced pressure. The crude solid residue was purified by silica gel flash column chromatography using cyclohexane/ethyl acetate (100:0 to 85:15) as eluent to afford the product as a white solid.

Preparation of Pybox ligand L2:



In a round bottom flask was placed at 0 °C the 2-amino-2-methyl-1-propanol (1.64 mL, 17.16 mmol, 3.5 equiv.) and NEt_3 (3.407 mL, 24.51 mmol, 5 equiv.) in DCM (16.5 mL) under an argon atmosphere. Then, a solution of pyridine dicarbonyl dichloride (1 g, 4.90 mmol, 1 equiv.) in DCM (8 mL) was added dropwise and the resulting solution was stirred for 16 h at room temperature. The reaction was washed with cold water (20 mL) and the aqueous phase was extracted with DCM (3 x 20mL). The combined organic phases were further washed with water (20 mL) and brine (20 mL). The organic phase was dried over $MgSO_4$ and concentrated under reduced pressure to afford the product **A** as a white solid which was used directly in the next step. In a round bottom flask, $SOCl_2$ (1.57 mL, 21.61 mmol, 6 equiv.) was added to a solution of 2-*N*,6-*N*-bis(1-hydroxy-2-methylpropan-2-yl)pyridine-2,6-dicarboxamide product **A** (1.11

g, 3.60 mmol, 1 equiv.) in toluene (14.4 mL, C = 0.25 M) under argon. The reaction was stirred under reflux for 16 h. The reaction was allowed to cool to 0 °C, then washed with saturated aqueous $NaHCO_3$ (20 mL). The aqueous phase was extracted with ethyl acetate (3 x 20 mL) and the combined organic phases were dried over $MgSO_4$ and concentrated under reduced pressure to afford the chlorinated product analogue of **A** as a yellow oil which was used directly in the next step. The oil residue was placed in a round bottom flask with anhydrous THF (22 mL, C = 0.2 M) and cooled at 0 °C. Then, NaH (866 mg, 21.70 mmol, 5 equiv.) was added portion-wise and the reaction was left to stir overnight at room temperature (monitored by TLC until the starting material was fully consumed). The reaction mixture was filtered through a pad of celite®, concentrated under reduced pressure and purified using silica gel flash column chromatography (cyclohexane/ethyl acetate/methanol from 50:50:0 to 0:90:10) to give the PyBox ligand **L2** as a slightly yellow solid (486 mg, 41 %).

General procedure for iron aziridination reaction:

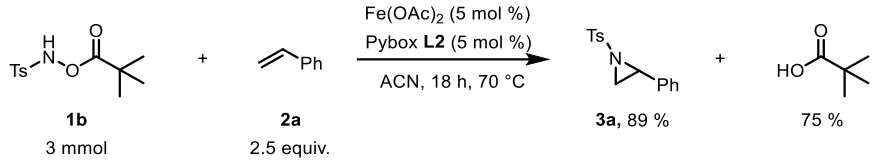
Procedure A: Aziridination for styrene derivatives:

The iron(II) acetate (0.027 mmol) and PyBox ligand **L2** (0.027 mmol) were placed in a sealed tube under argon. ACN (0.5 mL) was added to the tube and the suspension was stirred at room temperature for 10 mn. Then, the *N*-(acyloxy)-4-methylbenzenesulfonamide (0.27 mmol) substrate was added to the solution followed by the alkene partner (0.68 mmol) and ACN (0.9 mL). The tube was immediately sealed and stirred at 70 °C for 18 h. The reaction was quenched with a saturated aqueous solution of $NaHCO_3$, the aqueous phase was extracted with DCM (3x 20 mL). The combined organic phases were dried over $MgSO_4$ and concentrated under reduced pressure. The crude residue was purified by silica gel flash column chromatography (eluent: cyclohexane/ethyl acetate from 100:0 to 80:20) to afford the corresponding styryl aziridine.

Procedure B: Aziridination for alkyl alkenes:

The iron(II) triflate (0.02 mmol) and PyBox ligand **L2** (0.02 mmol) were placed in a sealed tube under argon. HFIP (0.5 mL) was added to the tube and the suspension was stirred at room temperature for 10 mn. Then, the *N*-(acyloxy)-4-methylbenzenesulfonamide (0.2 mmol) was added to the solution followed by the alkyl partner (0.5 mmol) and HFIP (0.5 mL). The tube was immediately sealed and placed at 50 °C to stir for 18 h. The reaction was quenched with a saturated aqueous solution of $NaHCO_3$, the aqueous phase was extracted using DCM (3x 20 mL). The combined organic phases were dried over $MgSO_4$ and concentrated under reduced pressure. The crude residue was purified by silica gel flash column chromatography (eluent: cyclohexane/ethyl acetate from 100:0 to 80:20) to afford the corresponding alkyl aziridine.

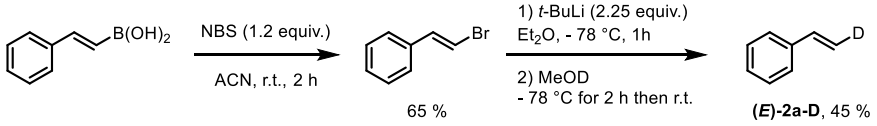
Large scale experiment:



In a round bottom flask, $Fe(OAc)_2$ (26 mg, 0.15 mmol, 0.05 equiv.) and Pybox ligand **L2** (40 mg, 0.15 mmol, 0.05 equiv.) were placed under argon in 15 mL of ACN (C = 0.2 M). The suspension was stirred at room temperature for 10 mn, then substrate **1b** (800 mg, 3 mmol, 1 equiv.) was added followed by styrene (0.85 mL, 7.40 mmol, 2.5 equiv.) and the flask was sealed and stirred at 70 °C for 18 h. The reaction was quenched with a saturated aqueous $NaHCO_3$ solution and the aqueous phase was extracted with DCM (3x 30 mL). The combined organic phases were dried over $MgSO_4$ and concentrated under reduced pressure. The crude residue was purified by silica gel flash column chromatography (eluent: cyclohexane/ethyl acetate from 100:0 to 80:20) to afford 720 mg (89 % yield) of tosylaziridine **3a** as a white solid. The aqueous phases were acidified to pH 1-2 using a 1 M aqueous HCl solution then extracted with DCM (3x 30 mL). The combined organic phases were dried over $MgSO_4$ and concentrated under reduced pressure to afford 225 mg (75 % yield) of pivalic acid as a white solid.

Preparation of deuterated styrenes:

Preparation of (*E*)-2a-D styrene:

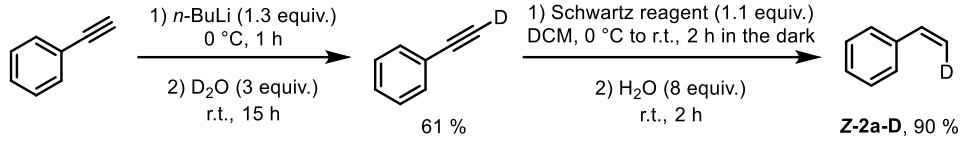


In a round bottom flask, to a solution of (*E*)-styryl-boronic acid (300 mg, 2.03 mmol, 1 equiv.) in acetonitrile (10.14 mL, C = 0.2 M) at room temperature was added NBS (433 mg, 2.43 mmol, 1.2 equiv.) in one portion. The reaction mixture was stirred vigorously for 2 h until complete consumption of boronic acid (monitored by TLC). The solution was then washed with an aqueous saturated $Na_2S_2O_5$ solution (20 mL) and the aqueous phase was extracted with pentane (3 x 20 mL). The combined organic layers were then washed with water (20 mL) dried over $MgSO_4$ and concentrated under reduced pressure to give (*E*)-2-bromostyrene as a yellow oil (240 mg, 65 %) without further purification.

In a round bottom flask, to a solution of (*E*)-2-bromostyrene (240 mg, 1.11 mmol, 1 equiv.) in anhydrous diethyl ether (5.3 mL, C = 0.2 M) at -78 °C was added carefully a solution of *t*-BuLi (C = 1.6 M in hexanes) (1.57 mL, 2.51 mmol, 2.25 equiv.) within a minute. The solution was

stirred at -78 °C for 1 h then methanol-d_4 (4.25 mL, 105 mmol, 94 equiv.) was added. The solution was allowed to warm to room temperature over 2 h, then stirred at room temperature for another 1 h. The reaction mixture was washed with an aqueous saturated NH_4Cl solution (20 mL) and the aqueous phase was extracted with diethyl ether (3 x 20 mL). The combined organic phases were washed with brine (20 mL) and dried over $MgSO_4$. The solvent was removed under reduced pressure without heating until approx. 5-10 mL of solvent was left over. Careful evaporation using a flow of air yielded **(***E***)**-2-deuterostyrene (**(*E*)-2a-D**) as a colorless oil (53 mg, 45 % yield, 100 % deuterated).

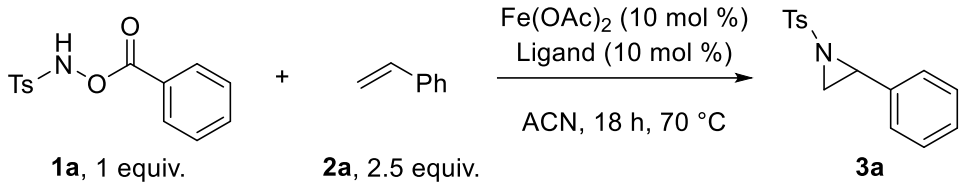
Preparation of (*Z*)-2a-D styrene:



In a round bottom flask, phenylacetylene (1.65 mL, 15 mmol, 1 equiv.) was added slowly to *n*-butyllithium (C = 1.6 M in hexanes) (12.2 mL, 19.53 mmol, 1.3 equiv.) over 15 minutes at 0 °C. The resulting suspension was stirred at 0 °C for 1 hour, then D_2O (1.11 mL, 41.6 mmol, 2.8 equiv.) was added slowly. The reaction was stirred at room temperature overnight, then passed through a pad of $MgSO_4$ washed with pentane and carefully concentrated under reduced pressure, without heating to afford phenylacetylene-d1 as a colorless liquid. In a round bottom flask, zirconocene hydrochloride (Schwartz' reagent) (1.1 g, 4.27 mmol, 1.1 equiv.) was added in two equal portions to a solution of phenylacetylene-d1 (400 mg, 3.9 mmol, 1 equiv.) in DCM (10 mL, C = 0.4 M) at 0 °C. After stirring at room temperature in the dark for 2 h, water (0.55 mL, 30.75 mmol, 8 equiv.) was added and the reaction was stirred for a further 2 h. The reaction was dried over $MgSO_4$, filtered and concentrated under reduced pressure to approx. 2 mL. Pentane (20 mL) was then added and the resulting solution was passed through a silica pad. Then the solid was washed with pentane and the filtrate was concentrated under reduced pressure (no heating) to afford (*Z*)-2-deuterostyrene (**(*Z*)-2a-D**) as a pale-yellow oil (367 mg, 90 % yield, 100 % deuterated).

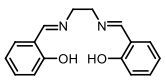
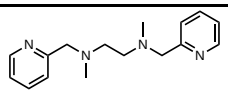
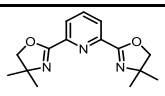
III. Optimization of reaction conditions

Optimization on styrene 2a:



1a, 1 equiv. **2a**, 2.5 equiv. **3a**

Table 1.

Entry	Ligand	Yield
1	---	25 %
2	Phenanthroline (20 mol%)	47 %
3	2,2’:6’,2’’-Terpyridine	13 %
4	2,2’-bipyridine (20 mol%)	trace
5		trace
6		trace
7	Tetraphenylporphyrin	7 %
8		80 %

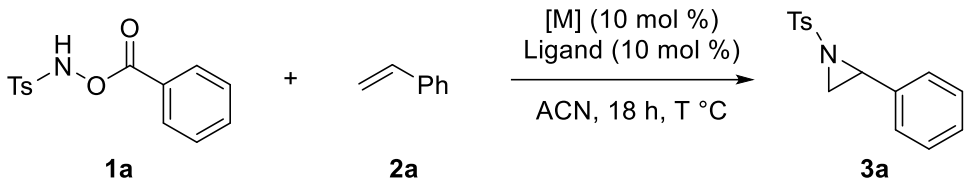
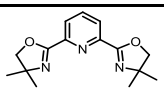
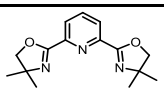
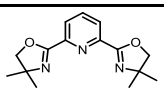
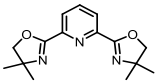
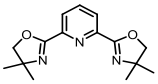
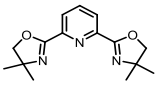
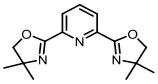
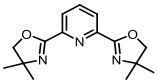
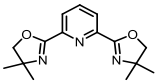
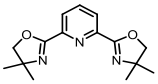


Table 2.

Entry	1 (equiv.)	2 (equiv.)	Fe Cat (10 mol%)	Ligand	T °C	Yield
1	1	2.5	$Fe(OTf)_2$		70 °C	23 %
2	1	2.5	$FeCl_2$		70 °C	47 %
3	1	2.5	$FeBr_3$		70°C	50 %
4	1	2.5	---	---	70 °C	0 %
5	1	2.5	$Cu(OAc)_2$		70 °C	trace
6	1	2.5	CuI		70 °C	trace
7	1	2.5	$Fe(OAc)_2$ (5 mol%)	 (5 mol%)	70 °C	78 %
8	1	2.5	$Fe(OAc)_2$		50 °C	76 %
9	1	2	$Fe(OAc)_2$		70 °C	77 %
10	1	1.5	$Fe(OAc)_2$		70 °C	63 %
11	2	1	$Fe(OAc)_2$		70 °C	58 %

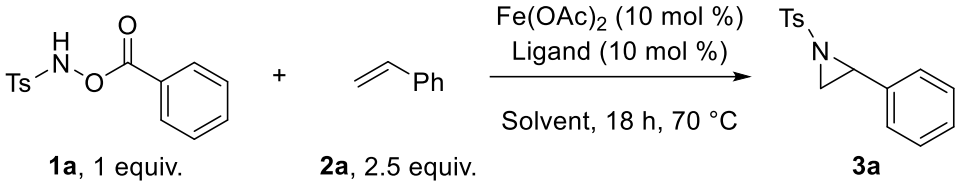
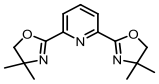
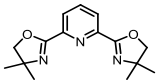
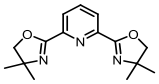
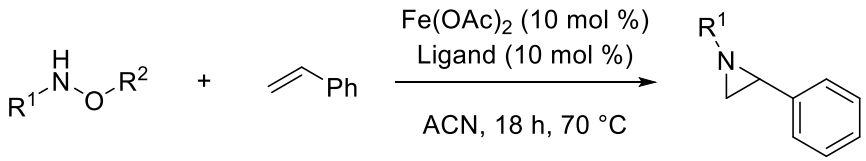


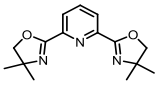
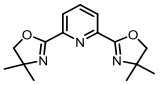
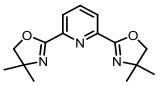
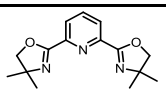
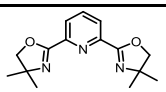
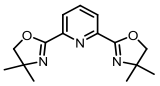
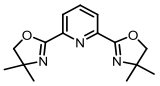
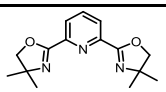
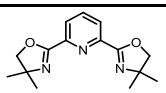
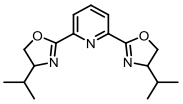
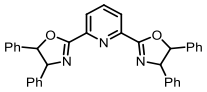
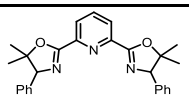
Table 3.

Entry	Ligand	Solvent	Yield
1		ACN	80 %
2		DCM/ACN 9:1	60 %
3		HFIP	0 %

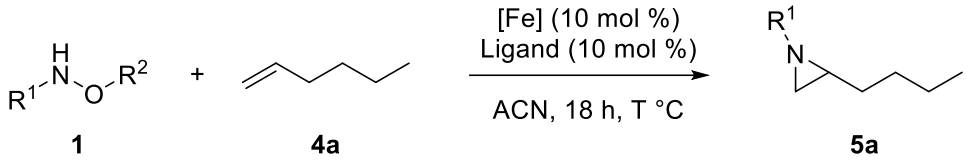


1a **2a** **3a**

Table 4.

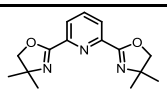
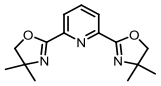
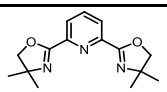
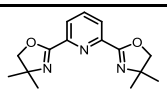
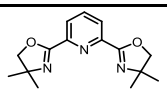
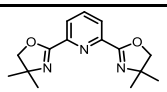
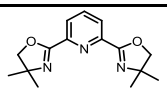
Entry	1 (equiv.)	2 (equiv.)	Ligand	R^1/R^2	Yield
1	1	2.5		Ns/Bz	60 %
2	1	2.5		Boc/Bz	0 %
3	1	2.5		Piv/Bz	0 %
4	1	2.5		Ts/Ac	0 %
5	1	2.5		Ts/4-nitrophenyl	0 %
6	1	2.5		Boc/4-nitrophenyl	0 %
7	1	2.5		Boc/2,4-dinitrophenyl	0 %
8	1	2.5		Ts/Piv	83 %
9	1	2		Ts/Piv	81 %
10	1	2.5		Ts/Piv	73 %
11	1	2.5		Ts/Piv	72 %
12	1	2.5		Ts/Piv	81 %

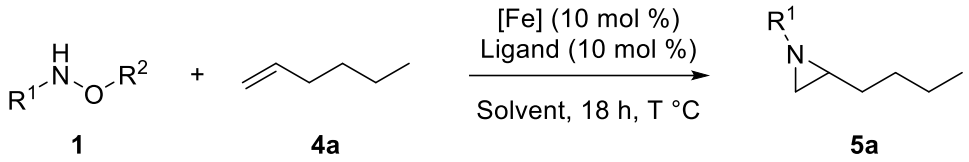
Optimization on hexene 4a:



1 **4a** **5a**

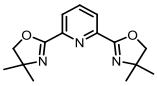
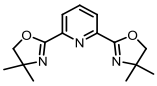
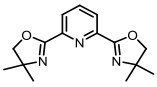
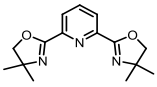
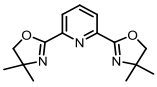
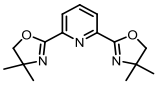
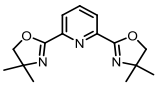
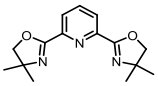
Table 5.

Entry	R^1/R^2	Fe Cat	Ligand	T °C	Yield
1	Ts/Piv	$Fe(OAc)_2$		50 °C	Trace
2	Ts/Piv	$Fe(OAc)_2$		70 °C	Trace
3	Ts/Piv	$Fe(OTf)_2$		70 °C	37 %
4	Ts/Piv	$Fe(OTf)_2$		50 °C	29 %
5	Ts/2,4-dichloro Bz	$Fe(OTf)_2$		70 °C	36 %
6	Ts/Bz	$Fe(OTf)_2$		70 °C	39 %
7	Ns/Bz	$Fe(OTf)_2$		70 °C	31 %
8	Ts/Piv	$Fe(OTf)_2$	Phenanth.	70 °C	Trace



1 **4a** **5a**

Table 6.

Entry	R^1/R^2	Fe Cat	Ligand	Solvent	T °C	Yield
1	Ts/Piv	$Fe(OTf)_2$		DCE	70 °C	25 %
2	Ts/Piv	$Fe(OTf)_2$		MeOH	70 °C	Trace
3	Ts/Piv	$Fe(OTf)_2$		THF	70 °C	0 %
4	Ts/Bz	$Fe(OTf)_2$		$MeNO_2$	70 °C	47 %
5	Ts/Bz	$Fe(OTf)_2$		HFIP	70 °C	58 %
6	Ts/Bz	$Fe(OTf)_2$		ACN / HFIP 4:1	70 °C	45 %
7	Ts/Bz	---	---	HFIP	70 °C	0 %
8	Ts/Bz	$Fe(OTf)_2$		HFIP	60 °C	62 %
9	Ts/Bz	$Fe(OTf)_2$		HFIP	50 °C	75 %

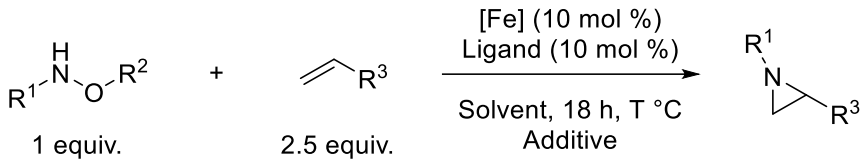
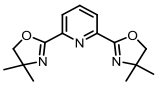
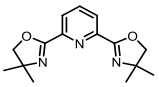
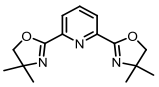
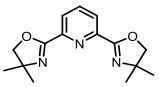
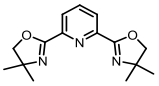
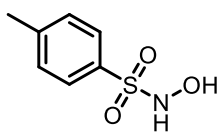


Table 7.

Entry	R^1/R^2	R^3	Fe Cat	Ligand	Solvent	Additive	T °C	Yield
1	Ts/Bz	Ph	$Fe(OAc)_2$		ACN	NaOAc (1 equiv.)	70 °C	0 %
2	Ts/Piv	C_4H_9	$Fe(OTf)_2$		ACN	K_2CO_3 (1 equiv.)	70 °C	0 %
3	Ts/Piv	C_4H_9	$Fe(OTf)_2$		ACN	NEt_3 (1 equiv.)	70 °C	0 %
4	Ts/Bz	C_4H_9	$Fe(OTf)_2$		HFIP	NEt_3 (10 mol %.)	r.t.	0 %
5	Ts/Bz	C_4H_9	$Fe(OTf)_2$		HFIP	Pyridine (10 mol %.)	r.t.	0 %

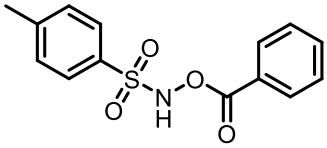
IV. Characterization of compounds

N-hydroxy-4-methylbenzenesulfonamide. Known compound[2]



white solid; m.p. 154-156 °C; ^{1}H NMR (MeOD, 500 MHz, ppm) δ = 7.82 (d, J = 8.5 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (MeOD, 125 MHz, ppm) δ = 145.4, 135.7, 130.4, 129.7, 21.5; IR (ν = cm^{-1}): 3386, 3221, 1595, 1319, 1157, 1089, 821, 725; HRMS (ESI): *m/z* calcd for $C_7H_8NO_3S$ [M - H$^+$] 186.0225, found 186.0226.

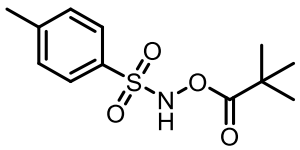
N-(benzoyloxy)-4-methylbenzenesulfonamide **1a**. Known compound[3]



1a

White solid; 90 % Yield; m.p. 91-94 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 9.21 (s, 1H), 7.92 (d, J = 8.5 Hz, 2H), 7.83 (d, J = 8.5 Hz, 2H), 7.63 (t, J = 7.5 Hz, 1H), 7.46 (t, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H);^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 165.1, 145.9, 134.7, 132.3, 130.1, 129.9, 129.0, 128.9, 125.9, 21.9; IR (ν = cm^{-1}): 3358, 3256, 3152, 1736, 1598, 1376, 1176, 1056, 815, 722; HRMS (ESI): *m/z* calcd for $C_{14}H_{12}NO_4S$ [M - H$^+$] 290.0487, found 290.0492.

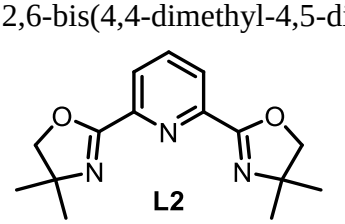
4-methyl-*N*-(pivaloyloxy)benzenesulfonamide **1b**. Known compound[4]



1b

White solid; 86 % Yield; m.p. 97-98 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 9.03 (s, 1H), 7.82 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 2.45 (s, 3H), 1.11 (s, 9H);^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 176.8, 145.9, 132.4, 130.0, 129.1, 38.4, 26.9, 21.9; IR (ν = cm^{-1}): 3134, 2982, 1754, 1358, 1170, 1101, 1086, 816, 752, 649; HRMS (ESI): *m/z* calcd for $C_{12}H_{18}NO_4S$ [M + H$^+$] 272.0957, found 272.0947.

2,6-bis(4,4-dimethyl-4,5-dihydrooxazol-2-yl)pyridine **L2**. Known compound[5]



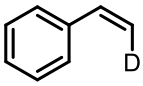
L2

Pale yellow to yellow solid; m.p. 130-132 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 8.18 (d, J = 7.5 Hz, 2H), 7.84 (t, J = 7.5 Hz, 1H), 4.21 (s, 4H), 1.39 (s, 12H);^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ =

[2] S.-M. Yang, B. Lagu, L. J. Wilson, *J. Org. Chem.* 2007, **72**, 8123.
[3] L. Fan, J. Hao, J. Yu, X. Ma, J. Liu, X. Luan, *J. Am. Chem. Soc.* 2020, **142**, 6698.
[4] A. Wang, J. Venditto, J. W. Darcy, M. H. Emmert, *Organometallics* 2017, **36**, 1259.
[5] D.-F. Lu, C.-L. Zhu, Z.-X. Jia, H. Xu, *J. Am. Chem. Soc.* 2014, **136**, 13186.

161.0, 147.1, 137.3, 125.8, 79.9, 68.2, 28.6; IR (ν = cm^{-1}): 3430, 2969, 2930, 2896, 1643, 1576, 1530, 1462, 1366, 1189, 1073, 975, 743; HRMS (ESI): *m/z* calcd for $C_{15}H_{20}N_3O_2$ [M + H^+] 274.1477, found 274.1545.

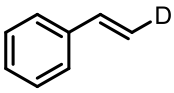
D-*cis*-styrene **(*Z*)-2a-D**. Known compound[6]



(*Z*)-2a-D

Colorless oil; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.41 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.27-7.25 (m, 1H), 6.71 (dt, *J* = 2.5 Hz, 10.5 Hz, 1H), 5.23 (d, *J* = 10.5 Hz, 1H).

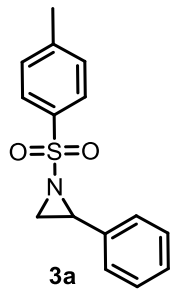
D-*trans*-styrene **(*E*)-2a-D**. Known compound[7]



(*E*)-2a-D

Colorless oil; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.41 (d, *J* = 7.0 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.27-7.25 (m, 1H), 6.72 (d, *J* = 17.5 Hz, 1H), 5.73 (d, *J* = 17.5 Hz, 1H).

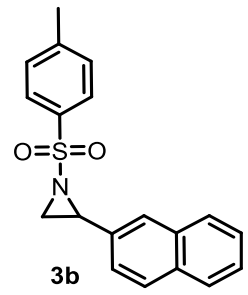
2-phenyl-1-tosylaziridine **3a**. Known compound.[8]



3a

White solid; m = 62 mg, 83 % Yield; m.p. 88-89 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.87 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.30-7.25 (m, 3H), 7.24-7.19 (m, 2H), 3.78 (dd, *J* = 4.5 Hz, 7 Hz, 1H), 2.99 (d, *J* = 7.5 Hz, 1H), 2.43 (s, 3H), 2.39 (d, *J* = 5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.8, 135.2, 129.9, 128.7, 128.4, 128.1, 126.7, 41.2, 36.0, 21.8; IR (ν = cm^{-1}): 3007, 2921, 1596, 1459, 1322, 1158, 1095, 909, 817, 781; HRMS (ESI): *m/z* calcd for $C_{15}H_{16}NO_2S$ [M + H^+] 274.0902, found 274.0889.

2-(naphthalene-2-yl)-1-tosylaziridine **3b**. Known compound[9]



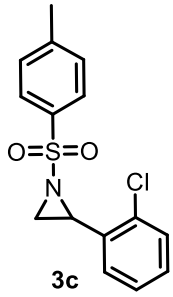
3b

White solid; m = 68 mg, 77 % Yield; m.p. 128-130 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.90 (d, *J* = 8.0 Hz, 2H), 7.81-7.75 (m, 3H), 7.73 (s, 1H), 7.50-7.43 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.26 (dd, *J* = 2.0 Hz, 8.5 Hz, 1H), 3.93 (dd, *J* = 4.5 Hz, 7.5 Hz, 1H), 3.07 (d, *J* = 7.5 Hz, 1H), 2.50 (d, *J* = 4.5 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.8, 135.2, 133.3, 133.2, 132.6, 129.9, 128.6, 128.1, 127.9, 127.8,

[6] L. T. Ball, G. C. Lloyd-Jones, C. A. Russell, *Chem. Eur. J.* 2012, **18**, 2931.
[7] R. Robiette, J. Pospisil, *Eur. J. Org. Chem.* 2013, 836.
[8] E. Martinand-Lurin, R. Gruber, P. Retailleau, P. Fleurat-Lessard, P. Dauban, *J. Org. Chem.* 2015, **80**, 1414.
[9] G.-Y. Gao, J. D. Harden, X. P. Zhang, *Org. Lett.* 2005, **7**, 3191.

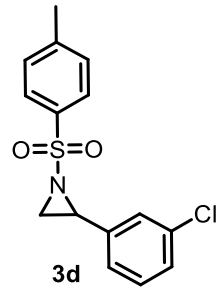
126.6, 126.4, 126.3, 123.8, 41.4, 36.1, 21.8; IR (ν = cm^{-1}): 3057, 2924, 2851, 1598, 1314, 1157, 1094, 926, 860, 820, 723; HRMS (ESI): *m/z* calcd for $C_{19}H_{18}NO_2S$ [M + H^+] 324.1058, found 324.1044.

2-(2-chlorophenyl)-1-tosylaziridine **3c**. Known compound[10]



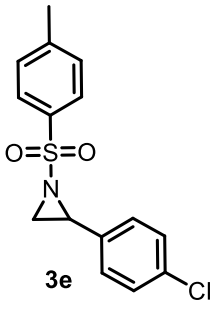
White solid; m = 74 mg, 87 % Yield; m.p. 92-93 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.90 (d, *J* = 7.5 Hz, 2H), 7.40-7.30 (m, 3H), 7.24-7.14 (m, 3H), 4.05 (brs, 1H), 3.04 (d, *J* = 7.0 Hz, 1H), 2.45 (s, 3H), 2.30 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 145.0, 134.7, 133.9, 133.2, 129.9, 129.4, 129.3, 128.3, 127.6, 127.1, 39.1, 35.8, 21.8; IR (ν = cm^{-1}): 2922, 1596, 1324, 1162, 1094, 907, 767, 731; HRMS (ESI): *m/z* calcd for $C_{15}H_{15}ClNO_2S$ [M + H^+] 308.0512, found 308.0499.

2-(3-chlorophenyl)-1-tosylaziridine **3d**. Known compound[4]



White solid; m = 72 mg, 85 % Yield; m.p. 59-60 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.86 (d, *J* = 8.5 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.27-7.20 (m, 2H), 7.18 (brs, 1H), 7.14-7.10 (m, 1H), 3.73 (dd, *J* = 4.5 Hz, 7.0 Hz, 1H), 2.97 (d, *J* = 7.0 Hz, 1H), 2.44 (s, 3H), 2.34 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 145.0, 137.4, 134.9, 134.7, 129.9, 128.6, 128.1, 126.7, 125.0, 40.2, 36.2, 21.8; IR (ν = cm^{-1}): 3068, 2922, 1605, 1320, 1310, 1156, 1092, 921, 837, 780, 727; HRMS (ESI): *m/z* calcd for $C_{15}H_{15}ClNO_2S$ [M + H^+] 308.0512, found 308.0499.

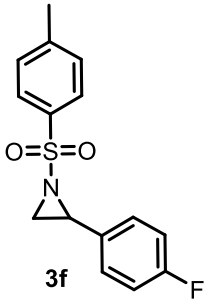
2-(4-chlorophenyl)-1-tosylaziridine **3e**. Known compound[11]



White solid; m = 74 mg, 87 % Yield; m.p. 112-113 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.85 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.28-7.24 (m, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 3.73 (dd, *J* = 4.0 Hz, 7.0 Hz, 1H), 2.98 (d, *J* = 7.5 Hz, 1H), 2.44 (s, 3H), 2.34 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.9, 135.0, 134.4, 133.8, 130.0, 128.9, 128.1, 128.0, 40.4, 36.2, 21.8; IR (ν = cm^{-1}): 2922, 1596, 1494, 1322, 1160, 1093, 912, 819, 732; HRMS (ESI): *m/z* calcd for $C_{15}H_{15}ClNO_2S$ [M + H^+] 308.0512, found 308.0499.

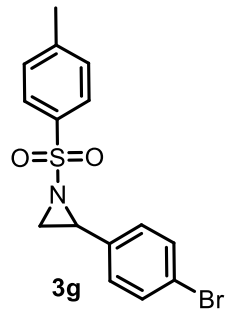
[10] Craig II, R. A.; O'Connor, N. R.; Goldberg, A. F. G.; Stoltz, B. M. *Chem. Eur. J.* **2014**, *20*, 4806.
[11] Hsueh, N.; Clarkson, G. J.; Shipman, M. *Org. Lett.* **2015**, *17*, 3632.

2-(4-fluorophenyl)-1-tosylaziridine **3f**. Known compound[3]



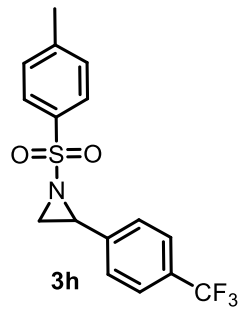
White oily paste; m = 67 mg, 84 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.86 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.21-7.16 (m, 2H), 6.97 (t, *J* = 8.5 Hz, 2H), 3.75 (dd, *J* = 4.5 Hz, 7.5 Hz, 1H), 2.96 (d, *J* = 7.0 Hz, 1H), 2.43 (s, 3H), 2.34 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 162.8 (d, *J* = 245 Hz), 144.9, 135.1, 131.0 (d, *J* = 3.6 Hz), 129.9, 128.4 (d, *J* = 8.1 Hz), 128.1, 115.7 (d, *J* =21.6 Hz), 40.4, 36.1, 21.8; IR (ν = cm^{-1}): 2924, 2849, 1597, 1515, 1338, 1158, 834, 816, 734; HRMS (ESI): *m/z* calcd for $C_{15}H_{15}FNO_2S$ [M + H^+] 292.0808, found 292.0794.

2-(4-bromophenyl)-1-tosylaziridine **3g**. Known compound[3]



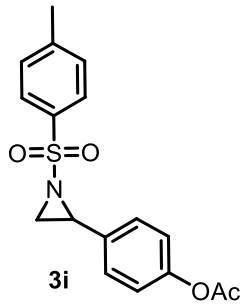
Isolated with a small amount of the debrominated aziridine. White solid; m = 74.5 mg, 77 % Yield; m.p. 120-122 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.85 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.5 Hz, 2H), 3.72 (dd, *J* = 4.5 Hz, 7.5 Hz 1H), 2.98 (d, *J* = 7.5 Hz, 1H), 2.44 (s, 3H), 2.34 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 145.0, 134.9, 134.3, 131.9, 129.9, 128.3, 128.1, 122.4, 40.5, 36.2, 21.8; IR (ν = cm^{-1}): 2922, 1596, 1489, 1319, 1160, 1093, 909, 821, 729; HRMS (ESI): *m/z* calcd for $C_{15}H_{15}BrNO_2S$ [M + H^+] 352.0007, found 351.9992.

1-tosyl-2-(4-(trifluoromethyl)phenyl)aziridine **3h**. Known compound[3]



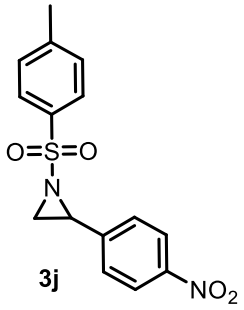
White solid; m = 65 mg, 70 % Yield; m.p. 79-82 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.87 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 4H), 3.81 (dd, J = 4.5 Hz, 7 Hz, 1H), 3.02 (d, *J* = 7.0 Hz, 1H), 2.44 (s, 3H), 2.37 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 145.1, 139.4, 134.9, 130.7 (q, *J* = 32.4 Hz), 130.0, 128.1, 127.1, 125.7 (d, *J* = 3.6 Hz), 124.0 (d, *J* = 270.4 Hz), 40.3, 36.3, 21.8; IR (ν = cm^{-1}): 2921, 2851, 1622, 1320, 1160, 1120, 1066, 918, 819, 713; HRMS (ESI): *m/z* calcd for $C_{16}H_{15}F_3NO_2S$ [M + H^+] 342.0776, found 342.0761.

4-(1-tosylaziridin-2-yl)phenyl acetate **3i**. Known compound[3]



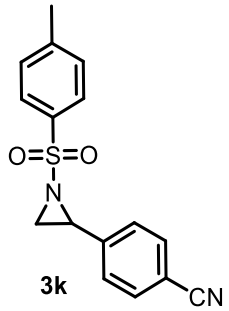
White solid; m = 71 mg, 78 % Yield; m.p. 96-100 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.86 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.01 (d, *J* = 8.5 Hz, 2H), 3.75 (dd, *J* = 4.5 Hz, 7.5 Hz, 1H), 2.98 (d, *J* = 7.0, 1H), 2.43 (s, 3H), 2.35 (d, *J* = 4.5 Hz, 1H), 2.27 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 169.5, 150.7, 144.9, 135.1, 132.8, 129.9, 128.1, 127.8, 121.9, 40.6, 36.1, 21.8, 21.2; IR (ν = cm^{-1}): 2921, 2849, 1759, 1510, 1320, 1220, 1191, 1156, 1092, 911, 815, 708; HRMS (ESI): *m/z* calcd for $C_{17}H_{16}NO_4S$ [M - H^+] 330.0800, found 330.0808.

2-(4-nitrophenyl)-1-tosylaziridine **3j**. Known compound[12]



White/yellowish solid; m = 52 mg, 59 % Yield; m.p. 108-112 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 8.15 (d, *J* = 9.0 Hz, 2H), 7.87 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 3.84 (dd, *J* = 4.5 Hz, 7.5 Hz, 1H), 3.05 (d, *J* = 7.5 Hz, 1H), 2.44 (s, 3H), 2.37 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 148.0, 145.3, 142.7, 134.6, 130.0, 128.1, 127.6, 124.0, 39.8, 36.7, 21.8; IR (ν = cm^{-1}): 3112, 3087, 2918, 2849, 1600, 1510, 1345, 1323, 1162, 898, 854, 724; HRMS (ESI): *m/z* calcd for $C_{15}H_{14}N_2O_4ClS$ [M + Cl^-] 353.0363, found 353.0369.

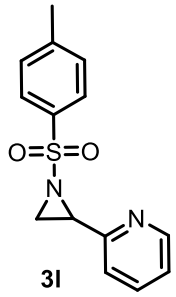
4-(1-tosylaziridine-2-yl)benzonitrile **3k**. Known compound[13]



White solid; m = 32 mg, 39 % Yield; m.p. 82-86 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.85 (d, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.34 (dd, *J* = 2.5 Hz, 8.5 Hz, 4H), 3.79 (dd, *J* = 4.0 Hz, 7.0 Hz, 1H), 3.01 (d, *J* = 7.0 Hz, 1H), 2.44 (s, 3H), 2.34 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 145.2, 140.7, 134.7, 132.5, 130.0, 128.1, 127.4, 118.5, 112.3, 40.0, 36.6, 21.8; IR (ν = cm^{-1}): 2927, 2849, 1597, 1453, 1320, 1162, 1094, 917, 815, 713; HRMS (ESI): *m/z* calcd for $C_{16}H_{15}N_2O_2S$ [M + H^+] 299.0854, found 299.0841.

[12] D. A. Evans, M. T. Bilodeau, M. M. Faul, *J. Am. Chem. Soc.* 1994, **116**, 2742.
[13] K. Kiyokawa, T. Kosaka, S. Minakata, *Org. Lett.* 2013, **15**, 4858.

2-(1-tosylaziridin-2-yl)pyridine **3l**. Known compound[4]

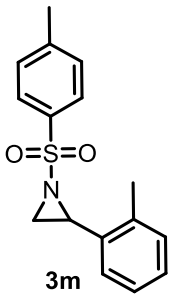


3l

This compound was prepared using aziridination procedure A with $Fe(OTf)_2$ (10 mol %) instead of $Fe(OAc)_2$ (10 mol %).

Yellow/orange oil; m = 20 mg, 27 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 8.52 (d, *J* = 5.0 Hz, 1H), 7.87 (d, *J* = 8.5 Hz, 2H), 7.63 (td, *J* = 2 Hz, 7.5 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 7.5 Hz, 1H), 7.22-7.18 (m, 1H), 3.90 (dd, *J* = 4 Hz, 7 Hz, 1H), 2.97 (d, *J* = 7.0 Hz, 1H), 2.66 (d, *J* = 4.5 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 154.5, 149.8, 144.9, 136.9, 134.8, 129.9, 128.3, 123.4, 121.9, 41.5, 35.1, 21.8; IR (ν = cm^{-1}): 2923, 1594, 1324, 1161, 1092, 914, 803, 714; HRMS (ESI): *m/z* calcd for $C_{14}H_{15}N_2O_2S$ [M + H$^+$] 275.0854, found 275.0841.

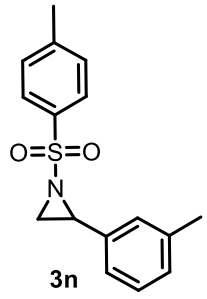
2-(*o*-tolyl)-1-tosylaziridine **3m**. Known compound[14]



3m

White solid; m = 66 mg, 83 % Yield; m.p. 78-80 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.91 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.21-7.09 (m, 4H), 3.87 (dd, *J* = 5 Hz, 7.5 Hz, 1H), 2.99 (d, *J* = 7.0 Hz, 1H), 2.45 (s, 3H), 2.39 (s, 3H), 2.32 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz, ppm) δ = 144.8, 136.8, 135.0, 133.3, 130.1, 129.9, 128.2, 128.1, 126.2, 126.0, 39.6, 35.1, 21.8, 19.2; IR (ν = cm^{-1}): 3057, 2918, 2845, 1597, 1460, 1321, 1161, 908, 773, 712; HRMS (ESI): *m/z* calcd for $C_{16}H_{18}NO_2S$ [M + H$^+$] 288.1058, found 288.1045.

2-(*m*-tolyl)-1-tosylaziridine **3n**. Known compound[3]

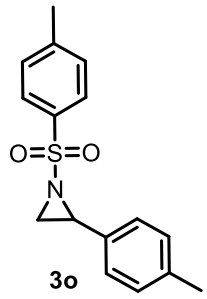


3n

White solid; m = 66 mg, 84 % Yield; m.p. 64-66 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.88 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 7.04-7.00 (m, 2H), 3.75 (dd, *J* = 4.5 Hz, 7.5 Hz, 1H), 2.96 (d, *J* = 7.0 Hz, 1H), 2.43 (s, 3H), 2.38 (d, *J* = 4.0 Hz, 1H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.7, 138.4, 135.1, 135.0, 129.9, 129.2, 128.6, 128.1, 127.2, 123.8, 41.1, 36.0, 21.8, 21.4; IR (ν = cm^{-1}): 3081, 2922 1596, 1453, 1317, 1156, 1091, 935, 863, 806, 788, 720; HRMS (ESI): *m/z* calcd for $C_{16}H_{18}NO_2S$ [M + H$^+$] 288.1058, found 288.1037.

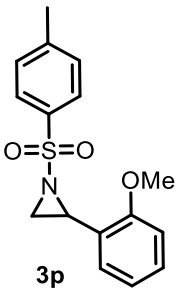
[14] C.-Y. Huang, A. G. Doyle, *J. Am. Chem. Soc*. 2012, **134**, 9541.

2-(*p*-tolyl)-1-tosylaziridine **3o**. Known compound[3]



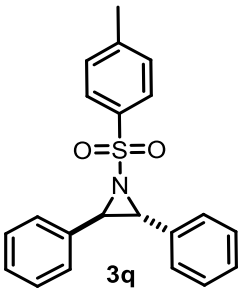
White solid; m = 58 mg, 73 % Yield; m.p. 133-134 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.86 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.1 (s, 4H), 3.74 (dd, *J* = 4.0 Hz, 1H), 2.97 (d, *J* = 7.0 Hz, 1H), 2.43 (s, 3H), 2.38 (d, *J* = 4.5 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.7, 138.3, 135.3, 132.2, 129.9, 129.4, 128.1, 126.6, 41.2, 35.9, 21.8, 21.3; IR (ν = cm^{-1}): 2920, 2851, 1595, 1518, 1319, 1159, 1093, 912, 815; HRMS (ESI): *m/z* calcd for $C_{16}H_{18}NO_2S$ [M + H^+] 288.1058, found 288.1043.

2-(2-methoxyphenyl)-1-tosylaziridine **3p**. Known compound[15]



White solid; m = 24 mg, 27 % Yield; m.p. 112-114 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.89 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.25-7.21 (m, 1H), 7.08 (dd, *J* = 2 Hz, 8 Hz, 1H), 6.89-6.79 (m, 2H), 4,07 (dd, *J* = 4.5 Hz, 7.5 Hz, 1H), 3.79 (s, 3H), 2.98 (d, *J* = 7.5 Hz, 1H), 2.44 (s, 3H), 2.33 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 158.2, 144.6, 135.2, 129.8, 129.3, 128.2, 126.7, 123.6, 120.7, 110.2, 55.5, 37.5, 35.3, 21.8; IR (ν = cm^{-1}): 3003, 2924, 2844, 1602, 1494, 1316, 1249, 1162, 910, 763, 715; HRMS (ESI): *m/z* calcd for $C_{16}H_{18}NO_3S$ [M + H^+] 304.1007, found 304.0993.

2,3-diphenyl-1-tosylaziridine **3q**. Known compound.[16]

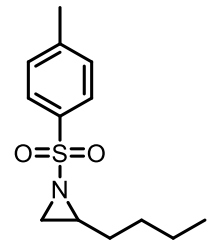


This compound was prepared using aziridination procedure A with a slight modification: substrate **1a** (0.4 mmol), $Fe(OAc)_2$ (5 mol %) and phenanthroline (10 mol %).

White solid; m = 70 mg, 50 % Yield; m.p. 136-138 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.63 (d, *J* = 8.5 Hz, 2H), 7.44-7.39 (m, 4H), 7.38-7.32 (m, 6H), 7.20 (d, *J* = 8.0 Hz, 2H), 4.26 (s, 2H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.1, 137.1, 133.1, 129.5, 128.8, 128.6, 128.4, 127.7, 50.5, 21.7; IR (ν = cm^{-1}): 3063, 2851, 1451, 1321, 1158, 903, 765; HRMS (ESI): *m/z* calcd for $C_{21}H_{18}NO_2S$ [M - H^+] 348.1058, found 348.1066.

[15] P.-J. Yang, L. Qi, Z. Liu, G. Yang, Z. Chai, *J. Am. Chem. Soc.* 2018, **140**, 17211.
[16] R. Vyas, G.-Y. Gao, J. D. Harden, X. P. Zhang, *Org. Lett.* 2004, **6**, 1907.

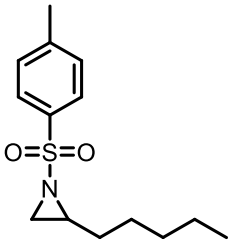
2-butyl-1-tosylaziridine **5a**. Known compound[8]



5a

Colorless oil; m = 38 mg, 75 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.82 (d, J = 8.5 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 2.75-2.68 (m, 1H), 2.62 (d, J = 6.5 Hz, 1H), 2.44 (s, 3H), 2.05 (d, J = 4.5 Hz, 1H), 1.57-1.49 (m, 1H), 1.38-1.32 (m, 1H), 1.27-1.20 (m, 4H) ,0.81 (t, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.5, 135.4, 129.7, 128.1, 40.5, 33.9, 31.1, 29.0, 22.2, 21.7, 13.9; IR (ν = cm^{-1}): 2958, 2930, 2861, 1598, 1457, 1323, 1160, 1091, 816, 714; HRMS (ESI): *m/z* calcd for $C_{13}H_{20}NO_2S$ [M + H$^+$] 254.1215, found 254.1203.

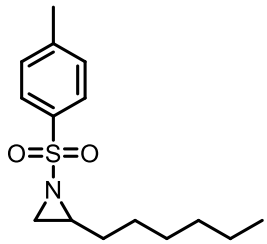
2-pentyl-1-tosylaziridine **5b**. Known compound[17]



5b

Colorless oil; m= 40 mg , 75 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.82 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 2.74-2.67 (m, 1H), 2.64 (d, J = 7.0 Hz, 1H), 2.44 (s, 3H), 2.06 (d, J = 4.5 Hz, 1H), 1.57-1.48 (m, 1H), 1.35-1.27 (m 1H), 1.23-1.16 (m, 6H), 0.82 (t, J = 6.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.6, 135.3, 129.8, 128.1, 40.7, 33.9, 31.4, 31.3, 26.6, 22.6, 21.8, 14.0; IR (ν = cm^{-1}): 2927, 2853, 1598, 1459, 1326, 1162, 1093, 930, 816, 715; HRMS (ESI): *m/z* calcd for $C_{14}H_{22}NO_2S$ [M + H$^+$] 268.1371, found 268.1365.

2-hexyl-1-tosylaziridine **5c**. Known compound[18]

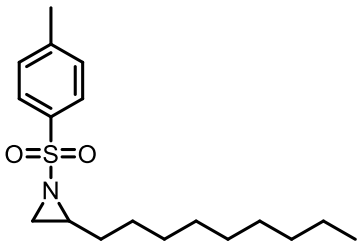


5c

Colorless oil; m = 41 mg, 73 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.83 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 2.74-2.68 (m, 1H), 2.64 (d, J = 7.0 Hz, 1H), 2.44 (s, 3H), 2.06 (d, J = 4.5 Hz, 1H), 1.57-1.50 (m, 1H), 1.34-1.29 (m, 1H), 1.23-1.13 (m, 8H), 0.85 (t, J = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.6, 135.3, 129.7, 128.1, 40.6, 33.9, 31.7, 31.5, 28.8, 26.9, 22.6, 21.8, 14.2; IR (ν = cm^{-1}): 2927, 2856, 1598, 1458, 1324, 1161, 1092, 714; HRMS (ESI): *m/z* calcd for $C_{15}H_{24}NO_2S$ [M + H$^+$] 282.1528, found 282.1515.

[17] D. M. Hodgson, M. J. Flemong, S. J. Stanway, *Org. Lett.* 2005, **15**, 3295.
[18] I. Saikia, B. Kashyap, P. Phukan, *Chem. Commun.*, 2011, **47**, 2967.

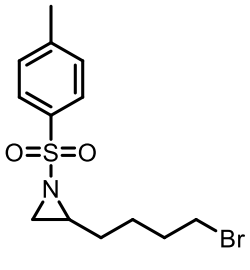
2-nonyl-1-tosylaziridine **5d**. Known compound[19]



5d

Colorless oil; m = 44.5 mg, 69 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.83 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 2.74-2.68 (m, 1H), 2.64 (d, J = 7.0 Hz, 1H), 2.44 (s, 3H), 2.05 (d, J = 4.5 Hz, 1H), 1.56-1.50 (m, 1H), 1.34-1.26 (m, 3H), 1.25-1.14 (m, 12H), 0.88 (t, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.5, 135.3, 129.7, 128.1, 40.7, 33.9, 32.0, 31.4, 29.5, 29.4, 29.2, 26.9, 22.8, 21.8, 14.3; IR (ν = cm^{-1}): 2956, 2929, 2854, 1597,1459, 1325, 1162, 1092, 925, 816, 715; HRMS (ESI): *m/z* calcd for $C_{18}H_{30}NO_2S$ [M + H$^+$] 324.1997, found 324.1991.

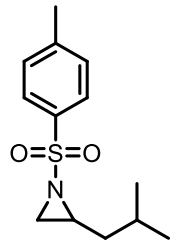
2-(4-bromobutyl)-1-tosylaziridine **5e**.



5e

Colorless oil; m = 41.5 mg, 62 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.83 (d, J = 8.5 Hz, 2H), 7.35 (d, J = 8.5 Hz, 2H), 3.31-3.26 (m, 2H), 2.74-2.68 (m, 1H), 2.65 (d, J = 7.0 Hz, 1H), 2.45 (s, 3H), 2.07 (d, J = 4.5 Hz, 1H), 1.81-1.74 (m, 2H), 1.67-1.60 (m, 1H), 1.41-1.27 (m, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.8, 135.1, 129.8, 128.1, 40.1, 33.9, 33.4, 32.0, 30.6, 25.6, 21.8; IR (ν = cm^{-1}): 3052, 2928, 2849, 1597, 1457, 1325, 1160, 1092, 915, 817, 768; HRMS (ESI): *m/z* calcd for $C_{13}H_{19}BrNO_2S$ [M + H$^+$] 332.0320, found 332.0314.

2-isobutyl-1-tosylaziridine **5f**. Known compound[20]

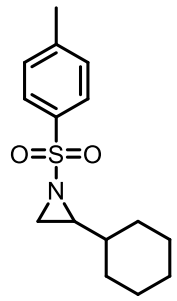


5f

Colorless oil; m = 43 mg, 84 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.82 (d, J = 8.5 Hz, 2H), 7.33 (d, J = 8.5 Hz, 2H), 2.82-2.74 (m, 1H), 2.62 (d, J = 7.5 Hz, 1H), 2.44 (s, 3H), 2.02 (d, J = 4.5 Hz, 1H), 1.63-1.56 (m, 1H), 1.37-1.29 (m, 2H), 0.88 (d, J = 2.5 Hz, 3H), 0.87 (d, J = 2.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.5, 135.3, 129.8, 128.1, 40.5, 39.2, 34.2, 26.9, 22.9, 22.0, 21.8; IR (ν = cm^{-1}): 2958, 2929, 2873, 1598, 1468, 1323, 1159, 1092, 870, 714; HRMS (ESI): *m/z* calcd for $C_{13}H_{20}NO_2S$ [M + H$^+$] 254.1215, found 254.1211.

[19] G. Kumaraswamy, K. Ankamma, A. Pitchaiah, *J. Org. Chem.* 2007, **72**, 9822.
[20] G. P. Y. Kok, H. Yang, M. W. Wong, Y. Zhao, *Org. Lett.* 2018, **20**, 5112.

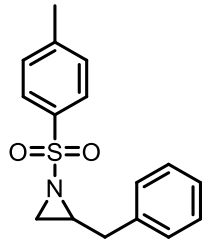
2-cyclohexyl-1-tosylaziridine **5g**. Known compound[21]



5g

Colorless oil; m = 33 mg, 59 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.82 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 2.59 (d, *J* = 7.0 Hz, 1H), 2.55-2.50 (m, 1H), 2.44 (s, 3H), 2.10 (d, *J* = 5.0 Hz, 1H), 1.72-1.66 (m, 1H), 1.66-1.59 (m, 3H), 1.53-1.47 (m, 1H), 1.17-0.99 (m, 5H), 0.96-0.87 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.5, 135.2, 129.7, 128.2, 45.3, 39.5, 32.8, 30.3, 29.7, 26.1, 25.7, 25.5, 21.8; IR (ν = cm^{-1}): 2926, 2852, 1598, 1450, 1323, 1160, 887, 720; HRMS (ESI): *m/z* calcd for $C_{15}H_{22}NO_2S$ [M + H^+] 280.1371, found 280.1367.

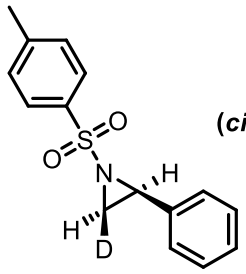
2-benzyl-1-tosylaziridine **5h**. Known compound[14]



5h

Colorless/White oily solid; m = 23 mg, 40 % Yield; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.69 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.5 Hz, 2H), 7.19-7.12 (m, 3H), 7.09-7.01 (m, 2H), 2.99-2.90 (m, 1H), 2.81 (dd, *J* = 5.5 Hz, 14.5 Hz, 1H), 2.74-2.66 (m, 2H), 2.42 (s, 3H), 2.16 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.4, 137.1, 134.9, 129.7, 128.8, 128.6, 128.0, 126.6, 41.3, 37.6, 33.0, 21.8; IR (ν = cm^{-1}): 3027, 2922, 2854, 1598, 1497, 1455, 1323, 1161, 714; HRMS (ESI): *m/z* calcd for $C_{16}H_{17}NO_2SNa$ [M + Na^+] 310.0878, found 310.0873.

2-phenyl-1-tosylaziridine-3-*d* **(*cis*)-3a-D**. Known compound[22]

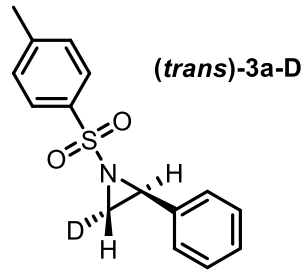


(*cis*)-3a-D

White solid; 81 % Yield (cis/trans ratio = 75:25); m.p. 84-85 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.87 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.30-7.27 (m, 3H), 7.24-7.20 (m, 2H), 3.78 (d, *J* = 7.0 Hz, 1H), 2.97 (d, *J* = 7.5 Hz, 1H, H-cis), 2.43 (s, 3H), [minor 2.38 (d, *J* = 4.5 Hz, 1H, H-trans)]; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.9, 135.2, 135.1, 130.0, 128.8, 128.5, 128.1, 126.8, 41.2, 35.9 (t, *J* = 27 Hz), 21.9.

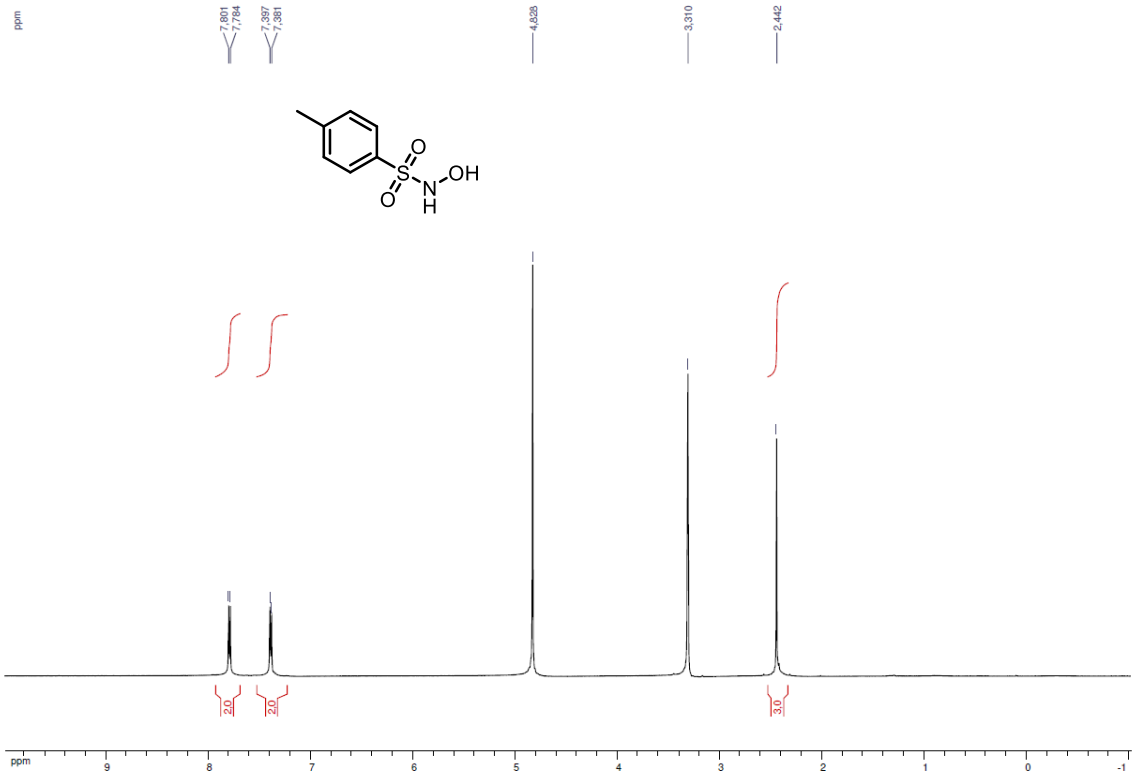
[21] J. M. Concellon, H. Rodriguez-Solla, C. Simal, *Org. Lett.* 2008, **10**, 4457.
[22] V. K. Aggarwal, E. Alonso, M. Ferrara, S. E. Spey, *J. Org. Chem.* 2002, **67**, 2335.

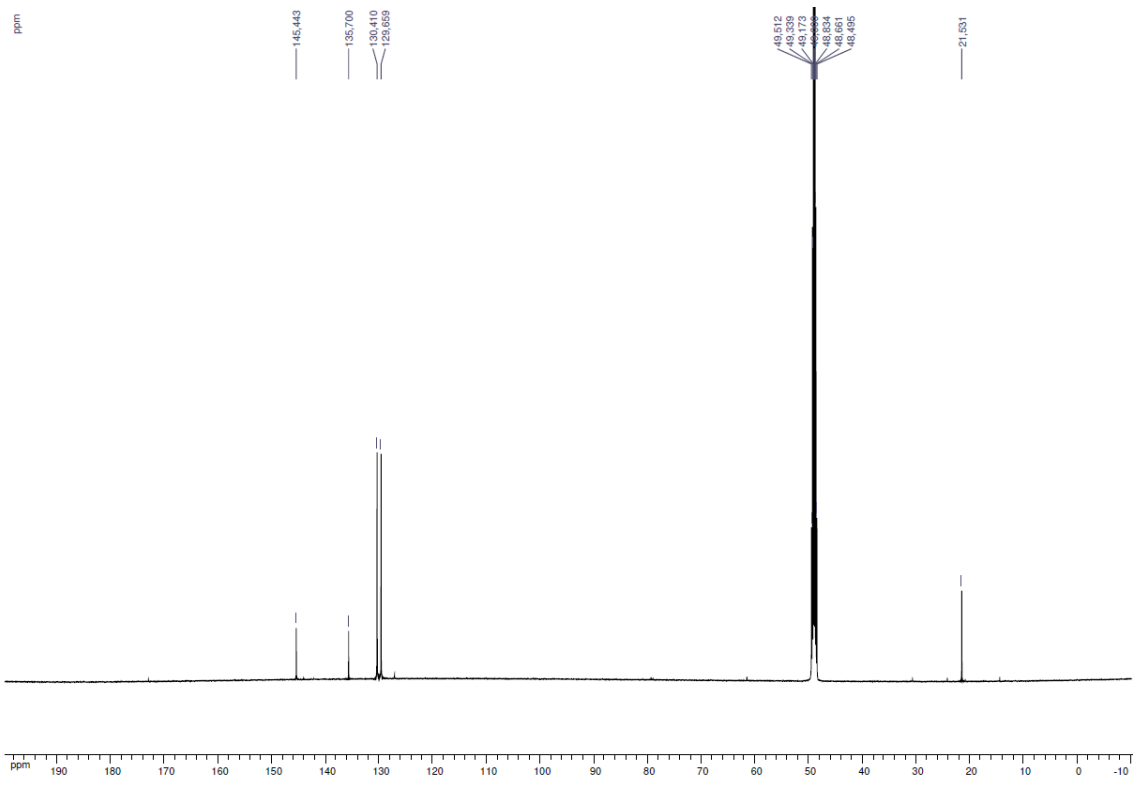
2-phenyl-1-tosylaziridine-3-*d* **(*trans*)-3a-D**.

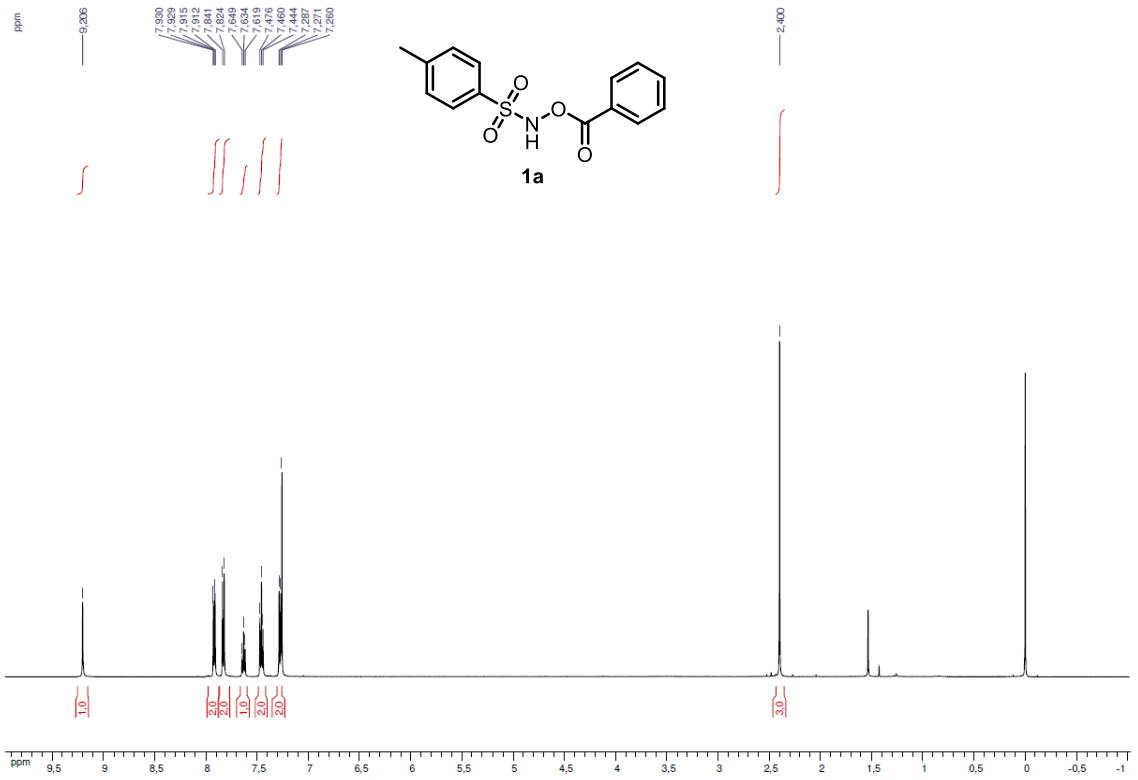


White solid; 78 % Yield (cis/trans ratio = 25:75); m.p. 84-85 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ = 7.87 (d, J = 8.5 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.30-7.27 (m, 3H), 7.24-7.20 (m, 2H), 3.77 (d, J = 5.0 Hz, 1H), [minor 2.97 (d, J = 7.5 Hz, 1H], H-cis), 2.43 (s, 3H), 2.38 (d, J = 4.5 Hz, 1H, H-trans); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ = 144.8, 135.2, 135.1, 129.9, 128.7, 128.4, 128.1, 126.7, 41.1, 35.8 (t, J = 25.7 Hz), 21.8.

V. Copy of ^{1}H and ^{13}C NMR spectra



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7,444
7,287
7,271
7,260
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3,0
ppm
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8,5
8
7,5
7
6,5
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4,5
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3,5
3
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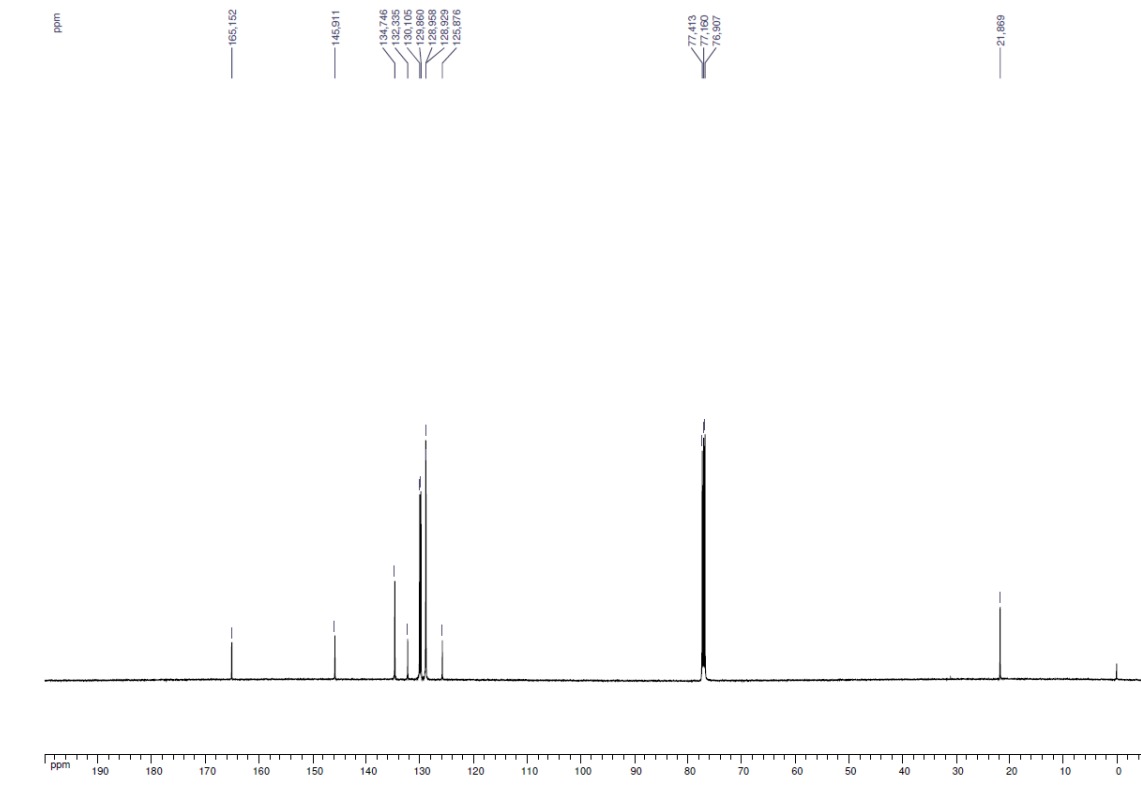
-1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ppm
190
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90
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70
60
50
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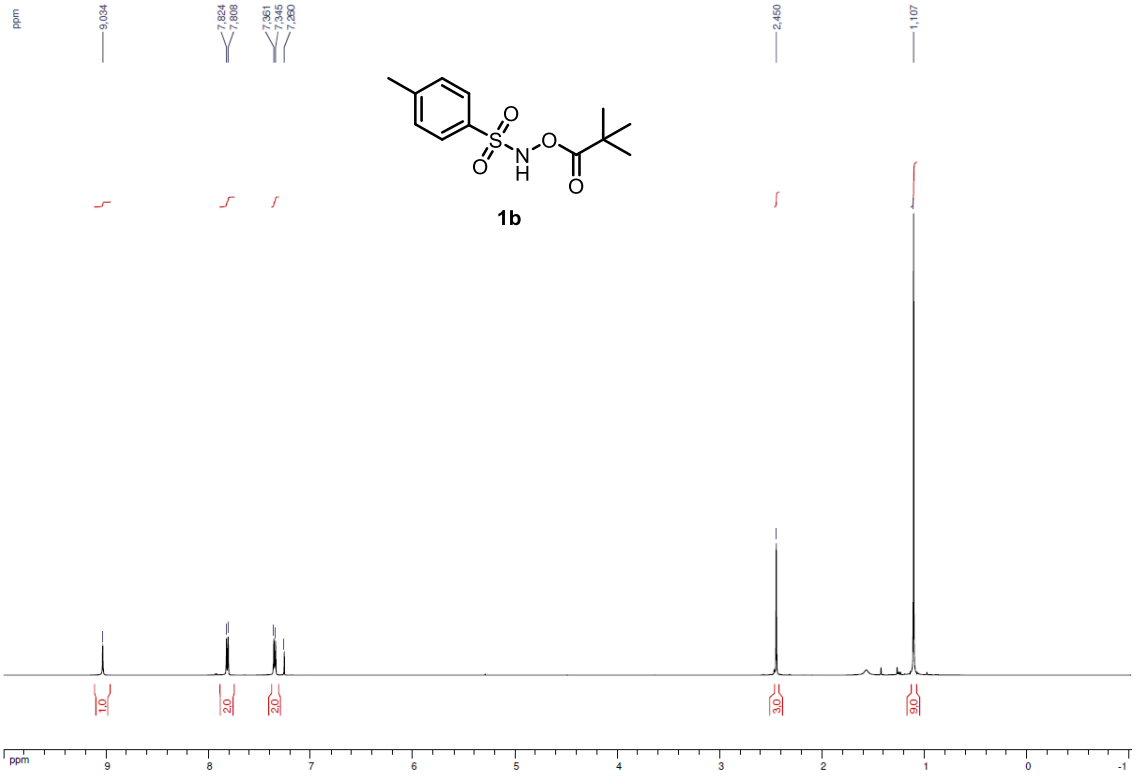
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6
5
4
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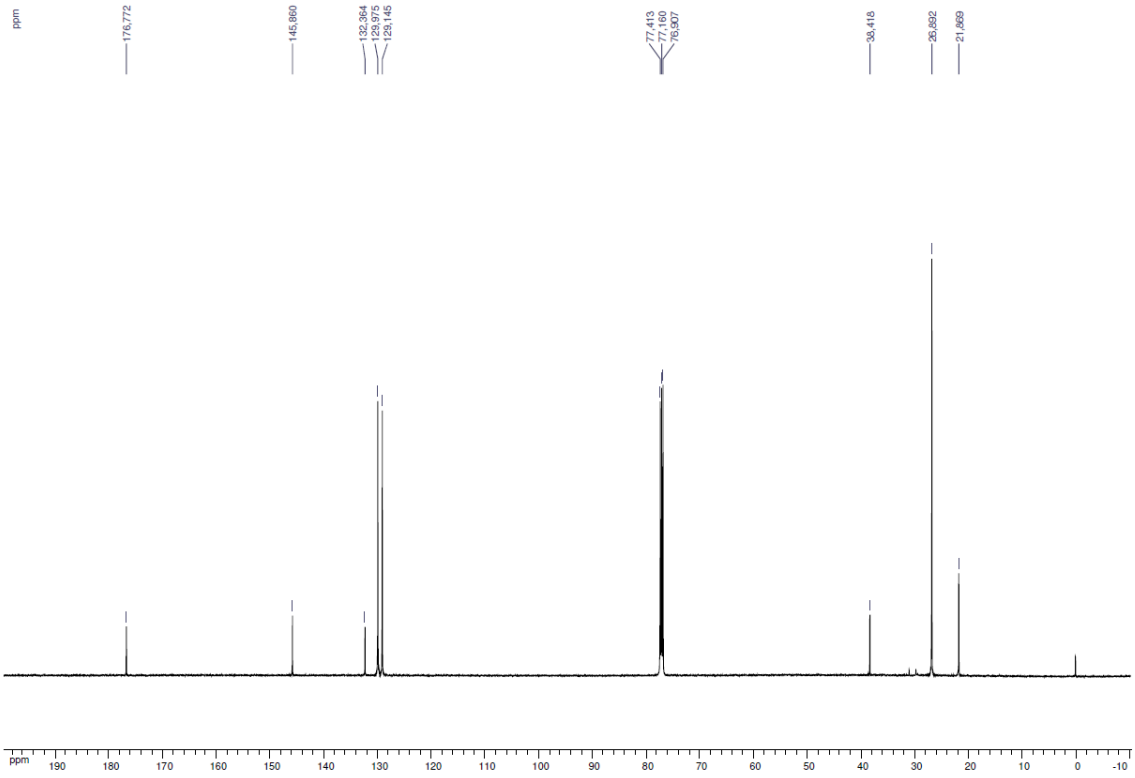
1b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26,892
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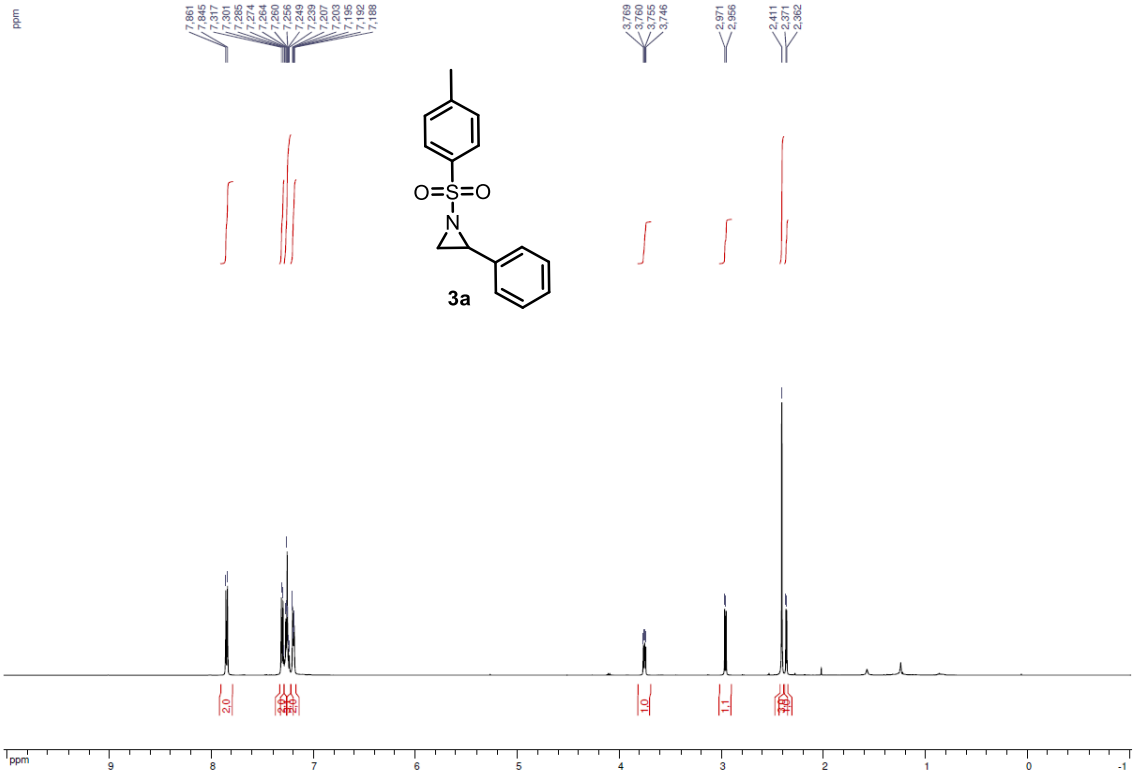
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7.285
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7.195
7.192
7.188
3.769
3.760
3.755
3.746
2.971
2.956
2.411
2.371
2.362
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N
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1.0
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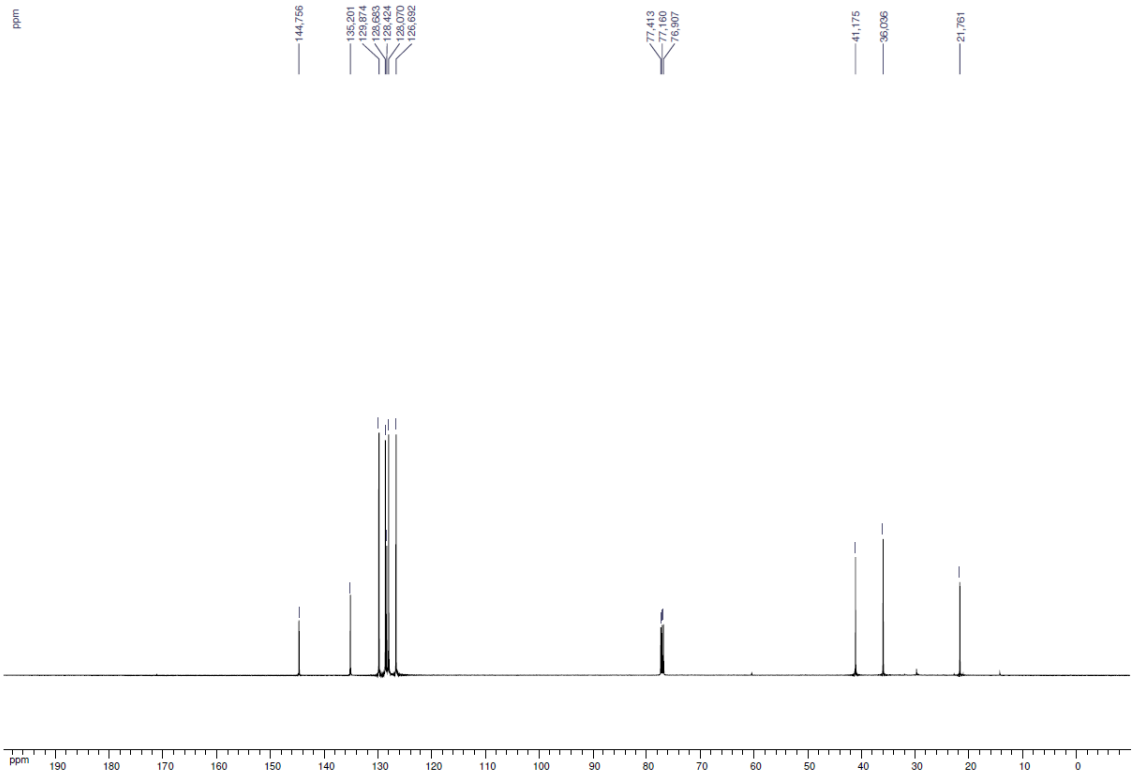
3a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77.160
76.907
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36.036
21.761
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120
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100
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80
70
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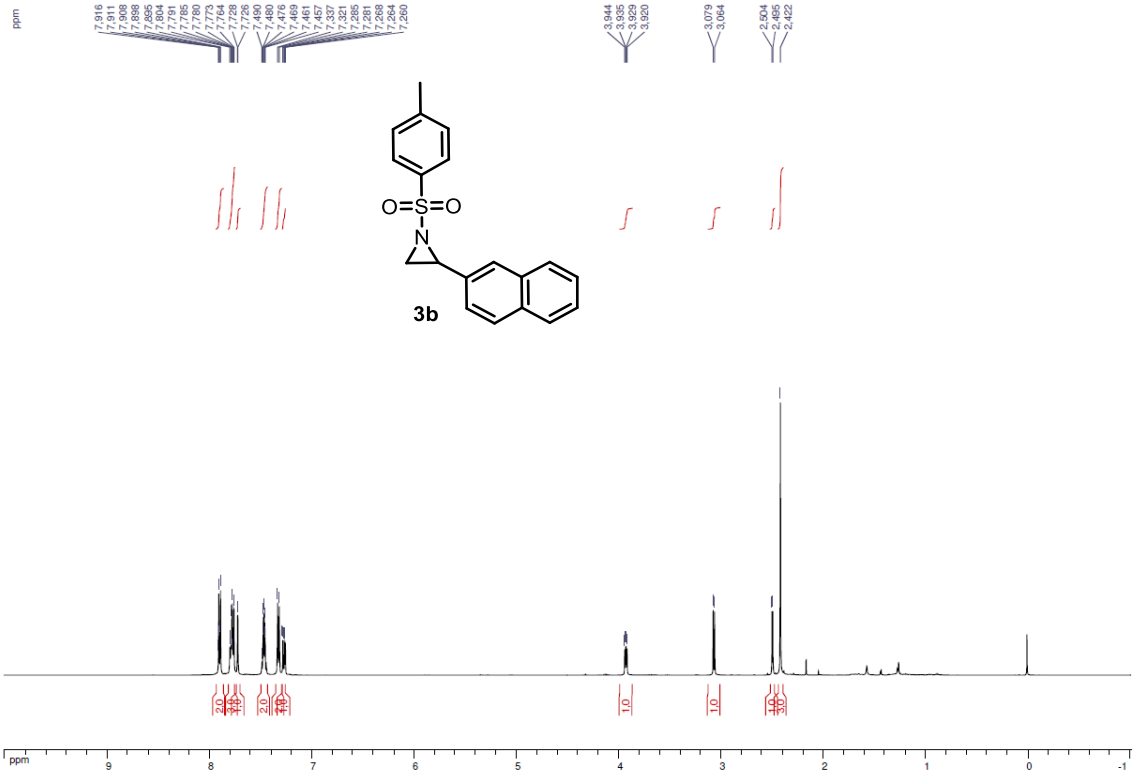
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7.490
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3.920
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3.064
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N
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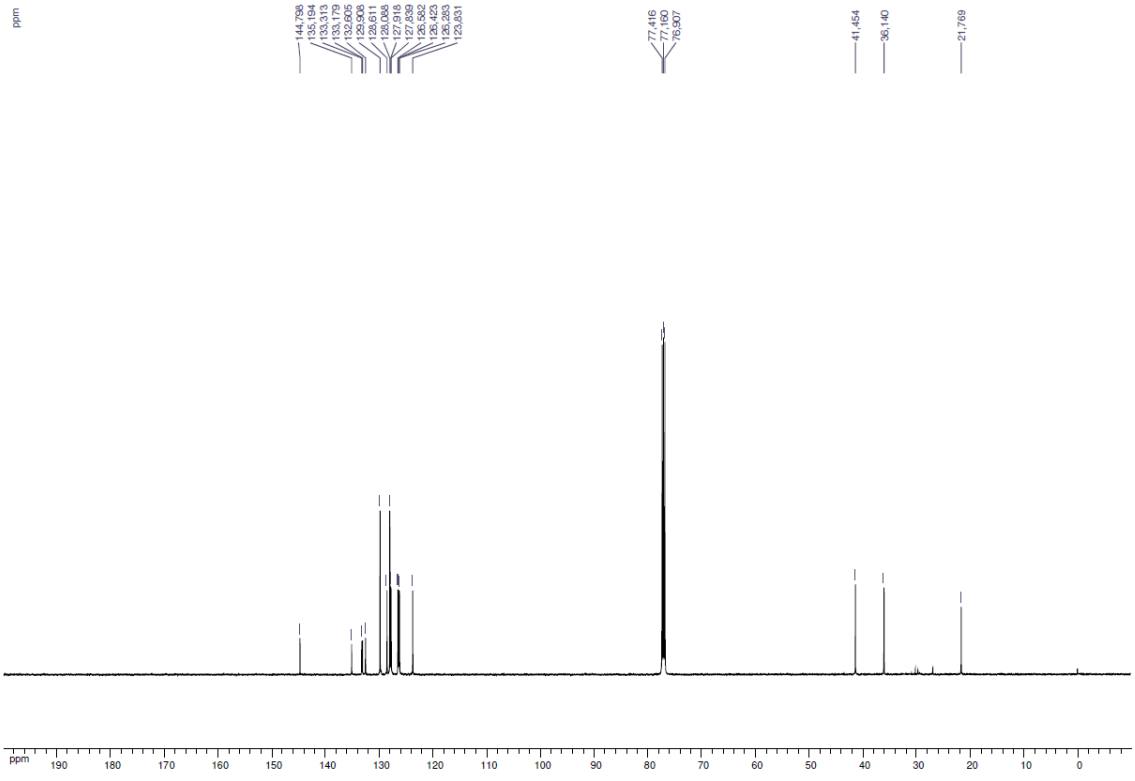
1.0
1.0
ppm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128.066
127.918
127.839
126.982
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126.263
123.631
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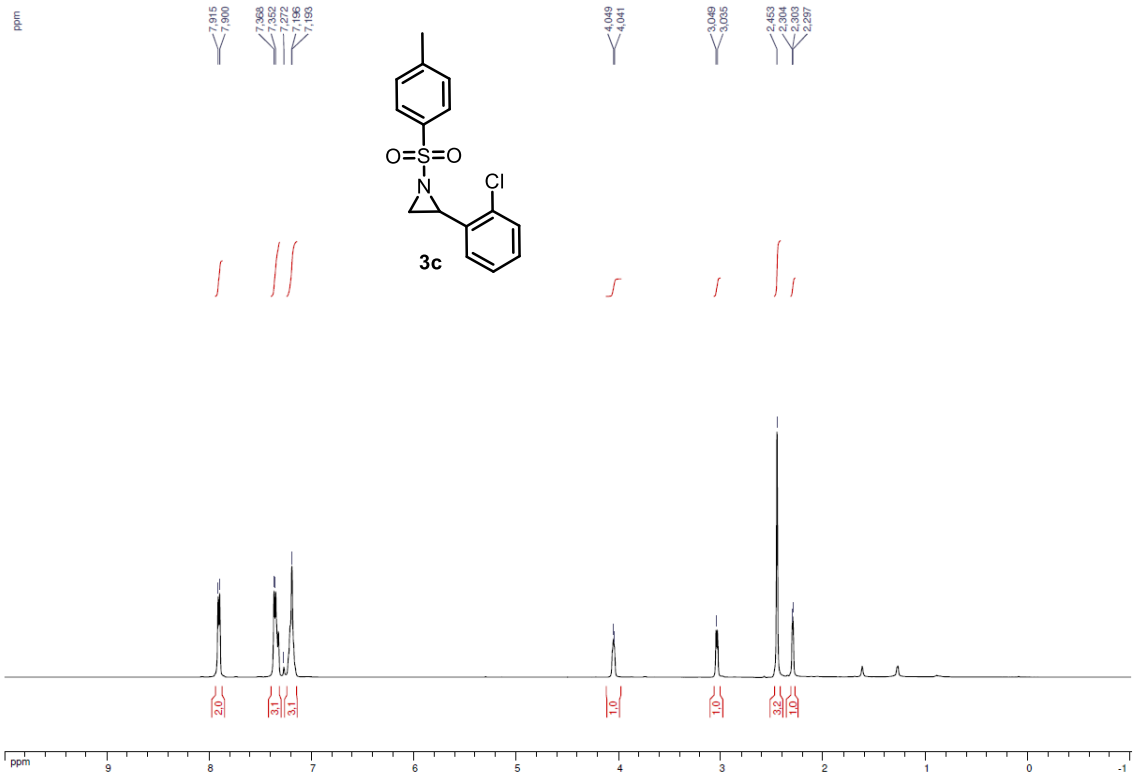
77.160
76.907
41.454
36.140
21.769
ppm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7.900
7.368
7.352
7.272
7.195
7.193
4.049
4.041
3.049
3.035
2.453
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2.303
2.297
O=S=O
N
Cl
3c
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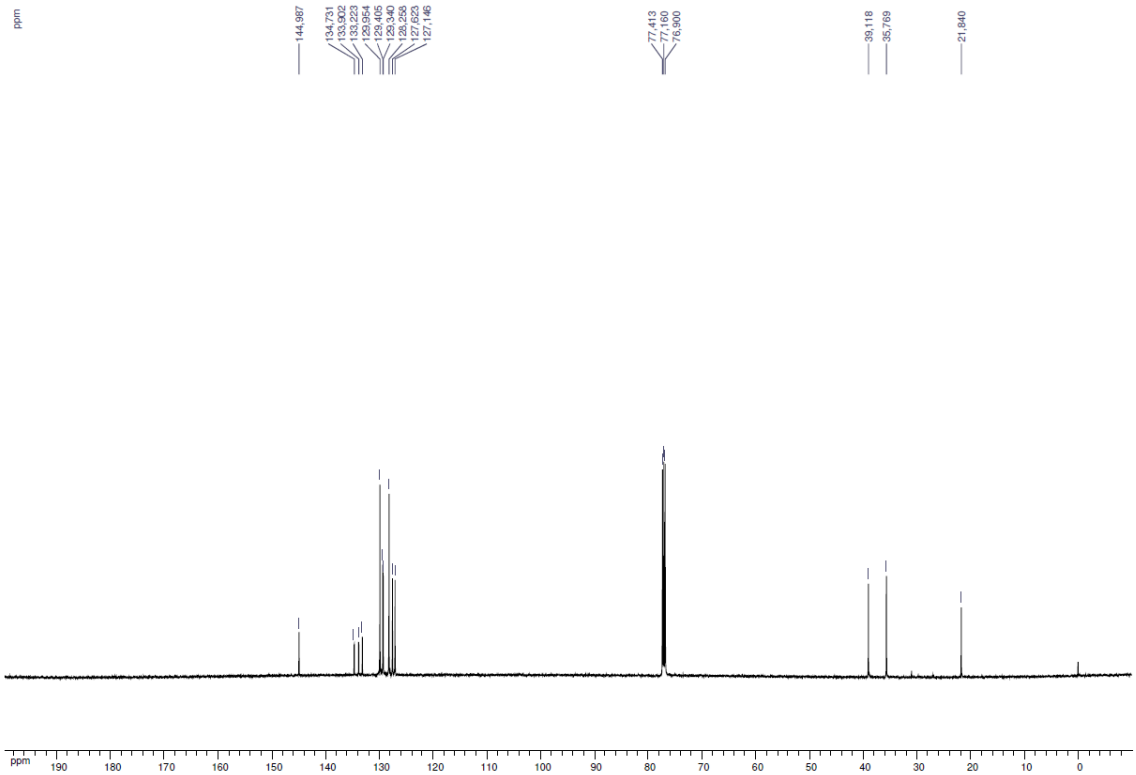
3.1
3.1
1.0
1.0
3.2
1.0
ppm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129.340
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127.146
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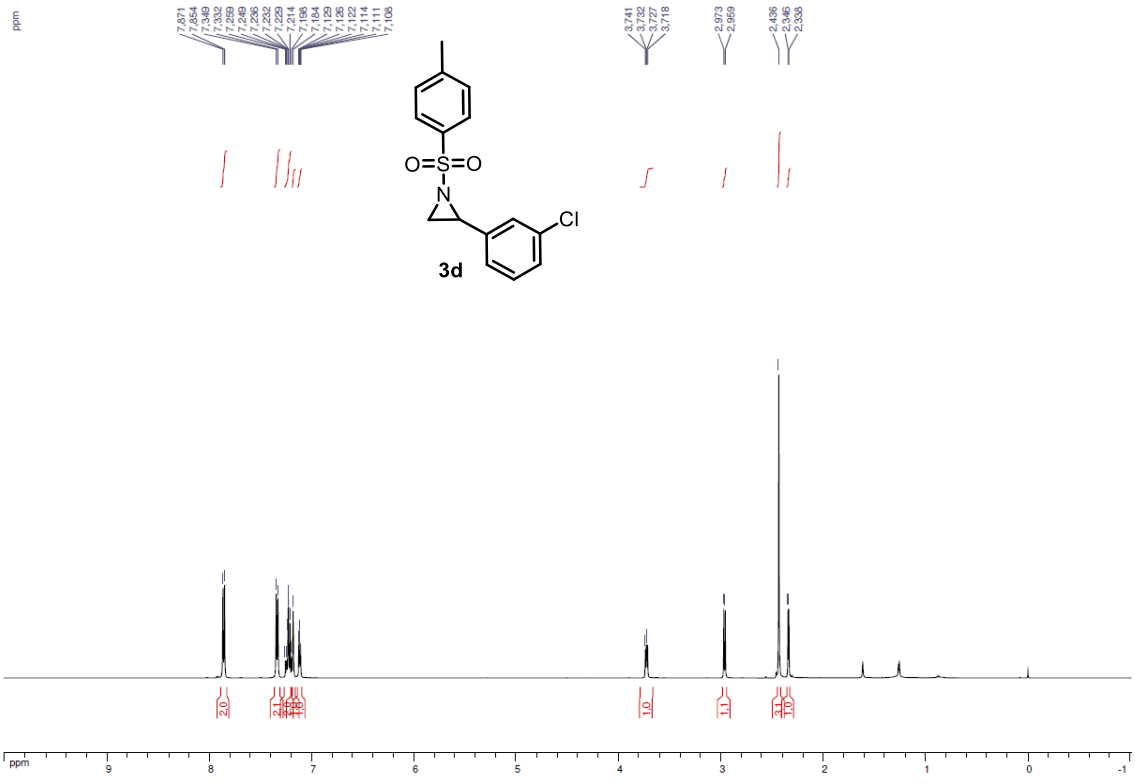
77.160
76.900
39.118
35.769
21.840
ppm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7.854
7.349
7.332
7.259
7.249
7.236
7.232
7.220
7.214
7.198
7.184
7.129
7.126
7.122
7.114
7.111
7.108
3.741
3.732
3.727
3.718
2.973
2.959
2.436
2.346
2.338
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N
Cl
3d
ppm
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8
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6
5
4
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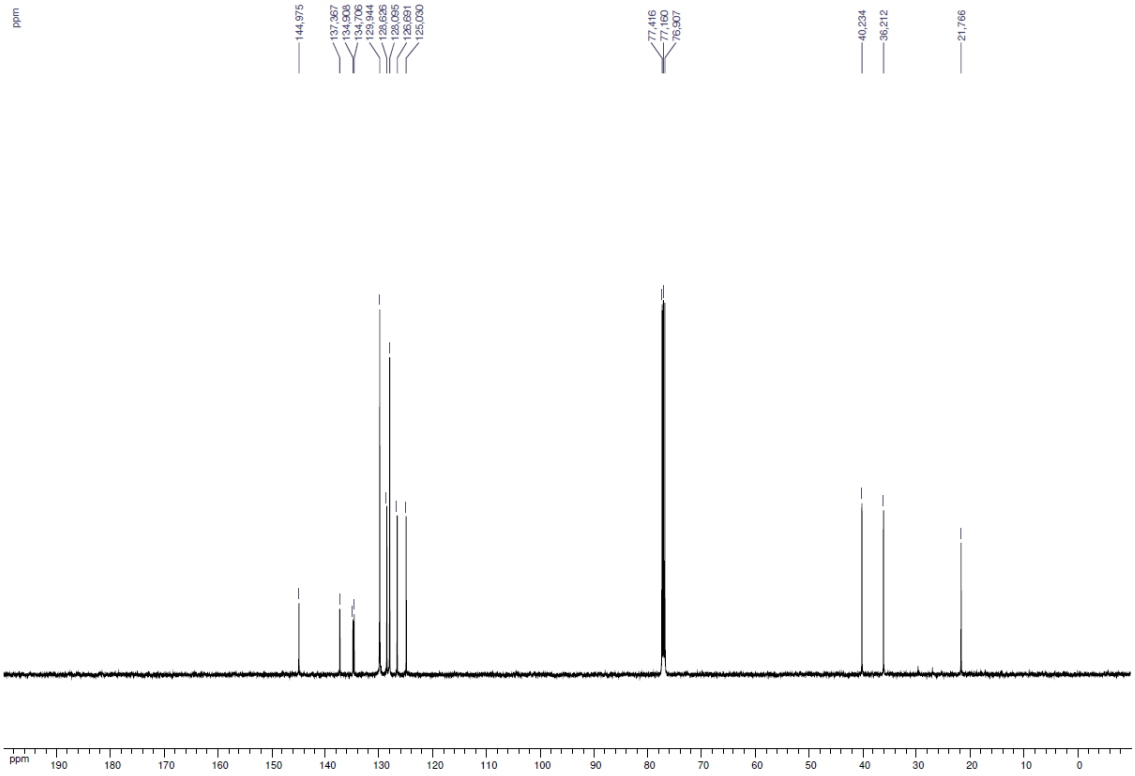
2
1
0
-1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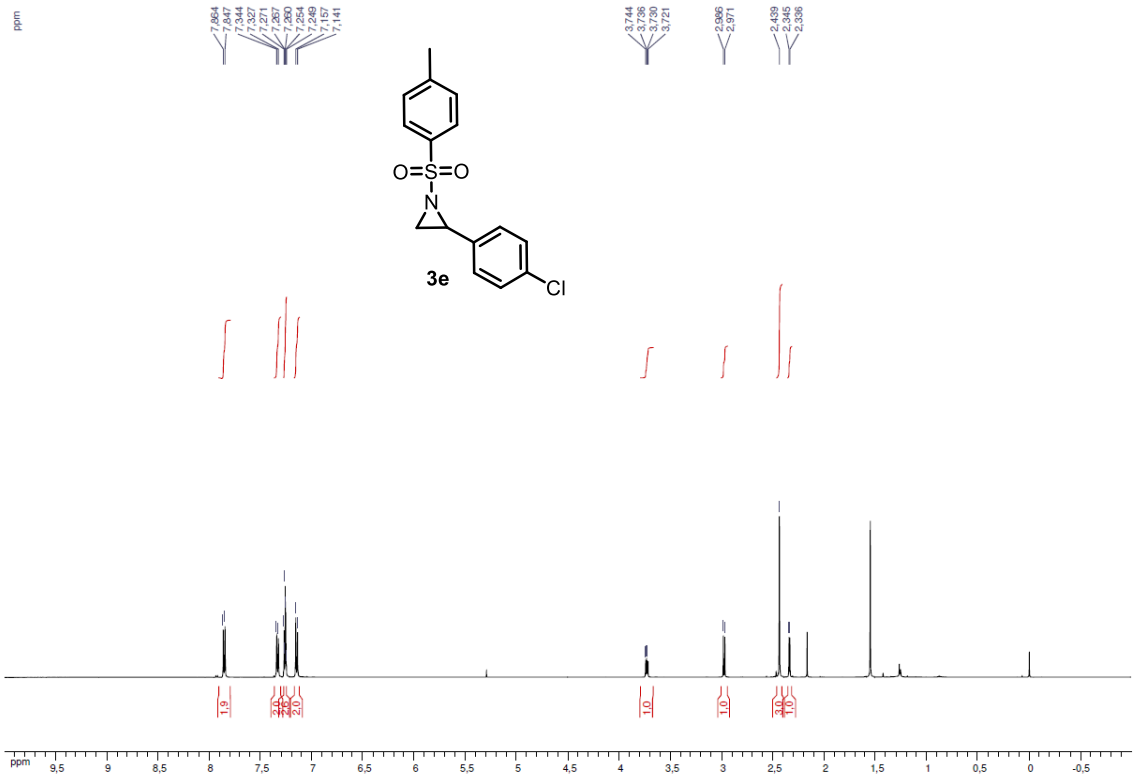
134.706
129.944
128.626
128.096
126.691
125.030
77.416
77.160
76.907
40.234
36.212
21.766
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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7,847
7,344
7,327
7,271
7,257
7,250
7,254
7,249
7,157
7,141
3,744
3,736
3,730
3,721
2,996
2,971
2,439
2,345
2,336
O=S=O
N
Cl
3e
1,9
2,0
2,0
2,0
1,0
1,0
1,0
1,0
ppm
9,5
9
8,5
8
7,5
7
6,5
6
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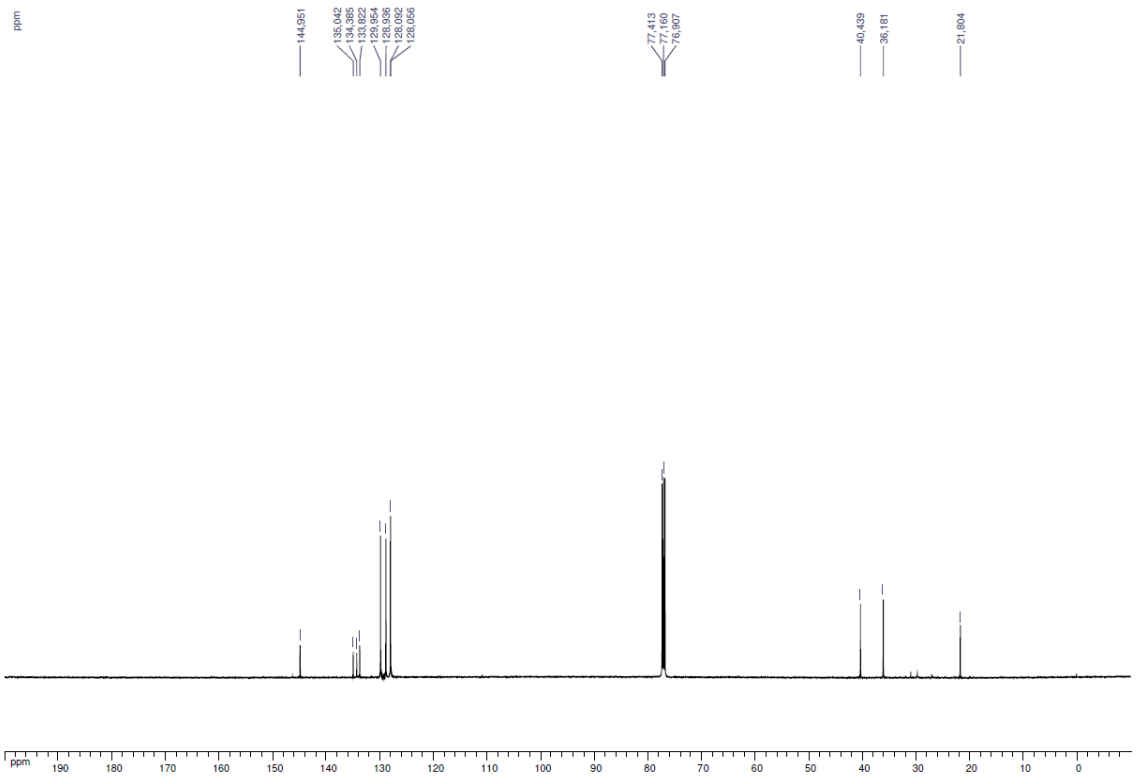
5
4,5
4
3,5
3
2,5
2
1,5
1
0,5
0
-0,5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134,395
133,822
129,954
128,936
128,092
126,056
77,413
77,160
76,907
40,439
36,181
21,804
ppm
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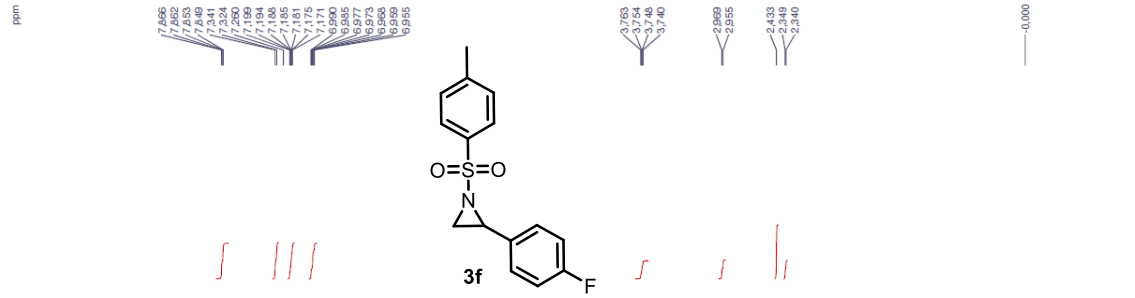
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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7,862
7,853
7,849
7,341
7,324
7,260
7,199
7,194
7,188
7,185
7,181
7,175
7,171
6,990
6,985
6,977
6,973
6,966
6,959
6,955
3,763
3,754
3,746
3,740
2,969
2,955
2,433
2,349
2,340
0,000
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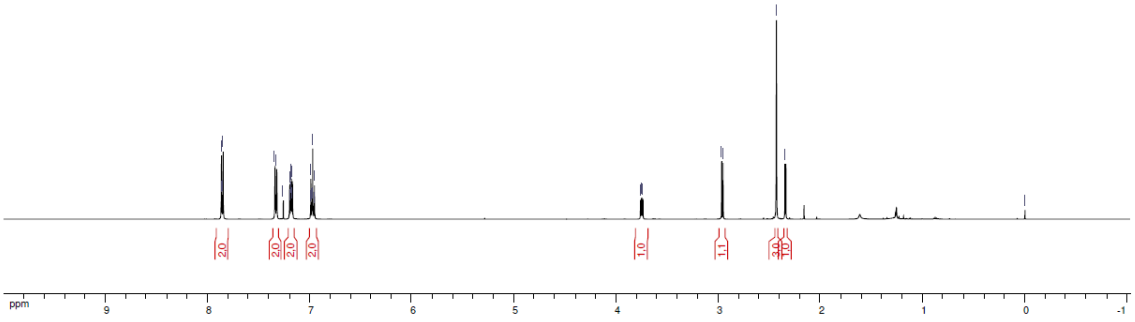
N
F
3f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2,0
2,0
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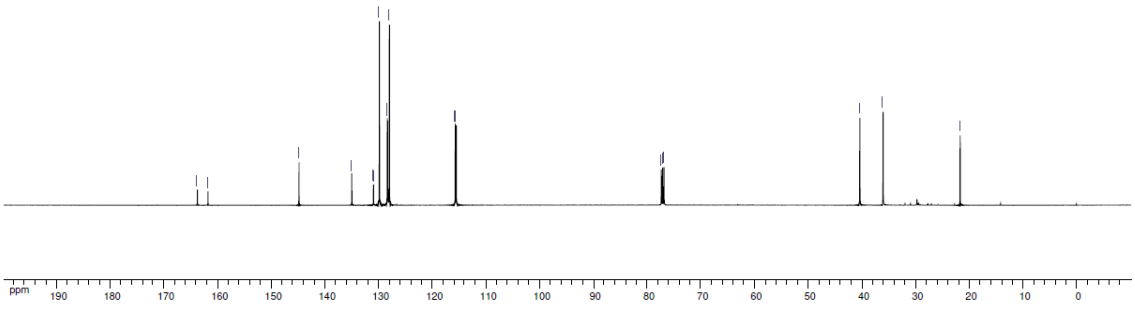
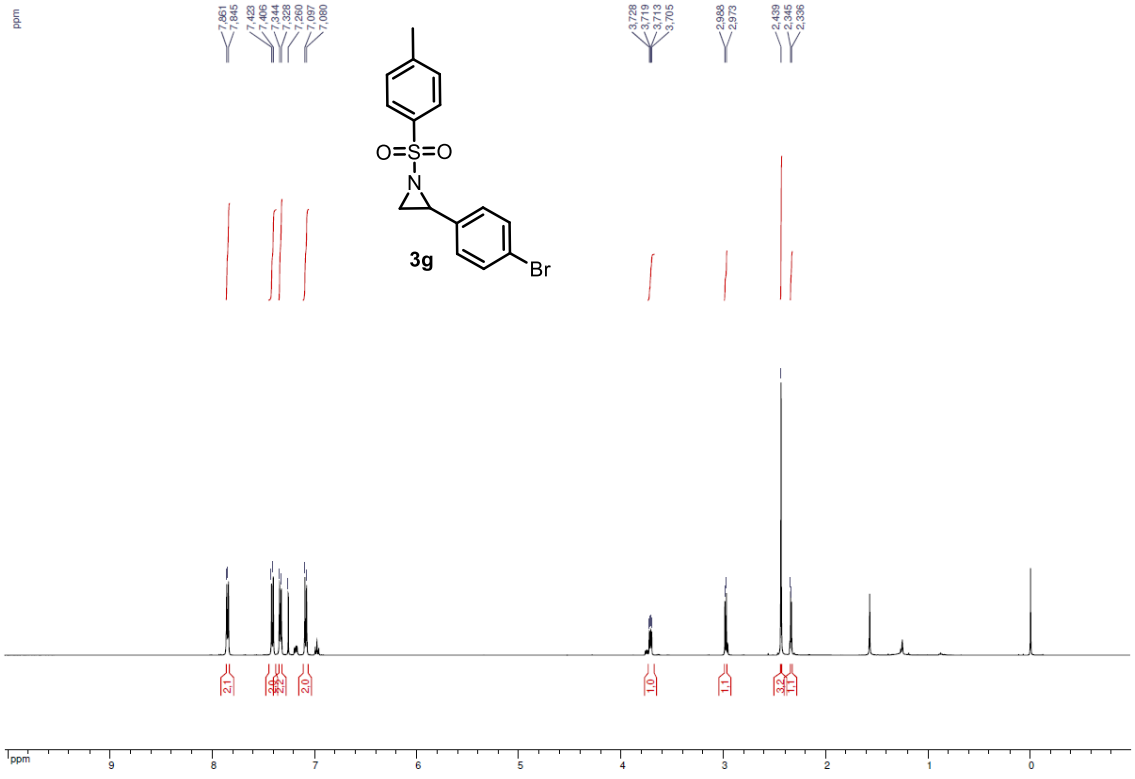
1,0
1,1
3,0
1,0
ppm
9
8
7
6
5
4
3
2
1
0
-1


ppm
163,802
161,389
144,879
135,063
131,022
130,993
129,010
128,453
128,398
128,063
115,779
115,606
77,413
77,160
76,907
40,446
36,123
21,768


ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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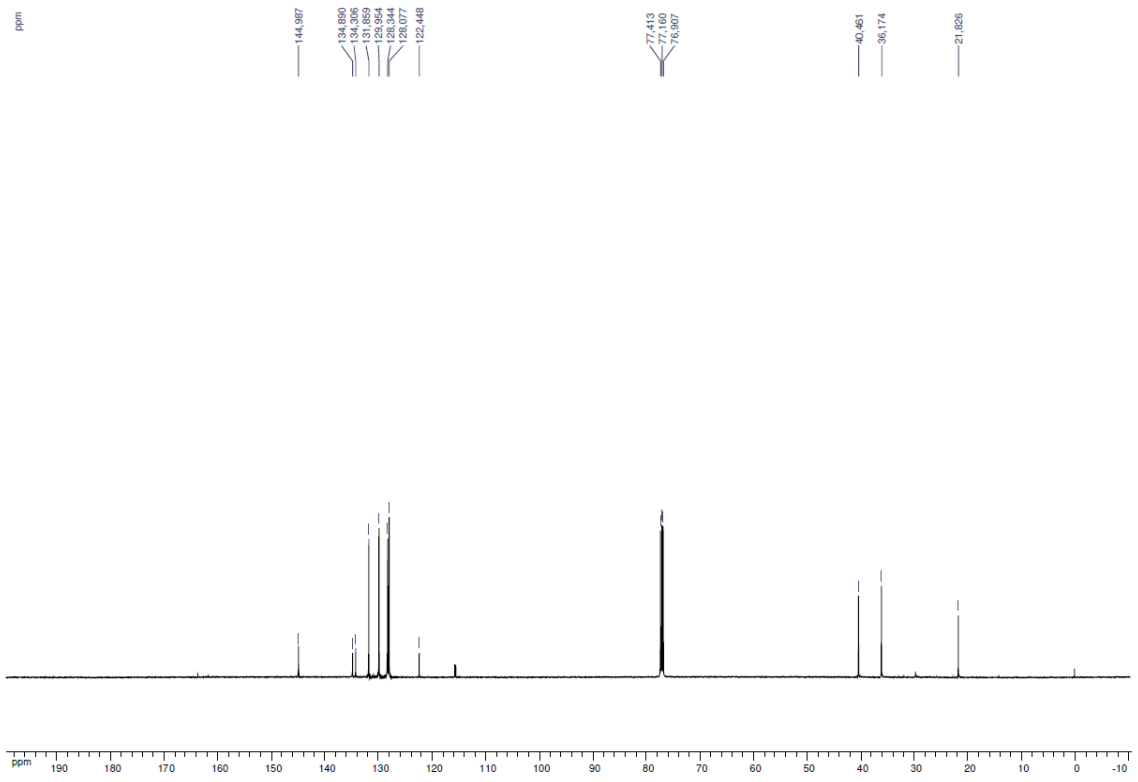
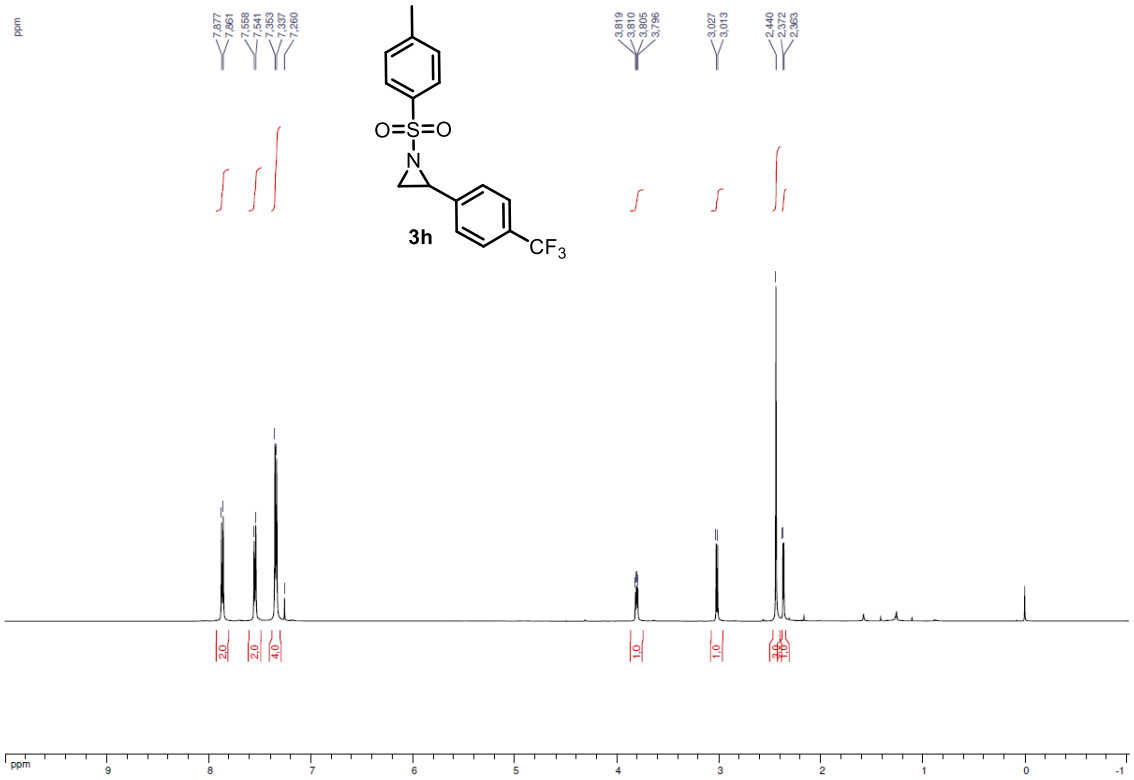
7.845
7.429
7.406
7.344
7.328
7.260
7.097
7.080
3.728
3.719
3.713
3.705
2.988
2.973
2.439
2.345
2.336
O=S=O
N
Br
3g
2.1
2.0
1.0
1.1
3.2
1.1
ppm


144.987
134.890
134.306
131.859
129.954
128.344
128.077
122.448
77.413
77.160
76.907
40.461
36.174
21.826
ppm


7,877
7,861
7,558
7,541
7,353
7,337
7,260
3,819
3,810
3,805
3,796
3,027
3,013
2,440
2,372
2,363
O=S=O
N
3h
CF3
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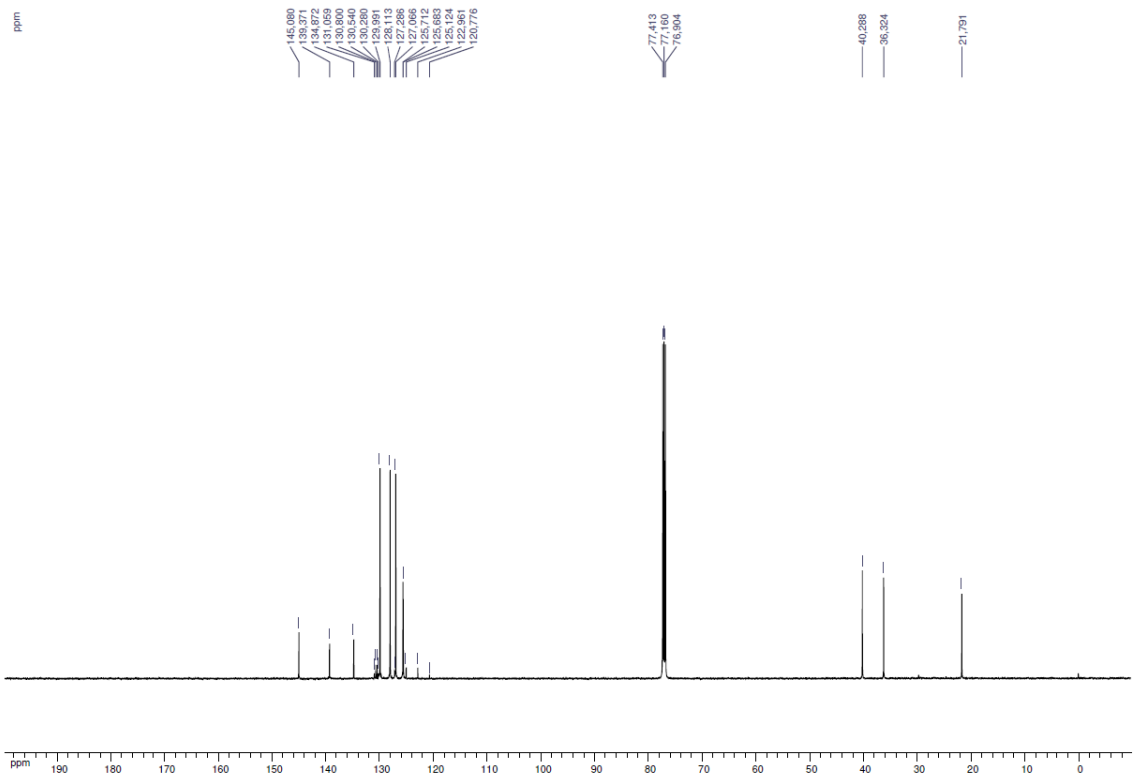
2.0
4.0
1.0
1.0
3.0
ppm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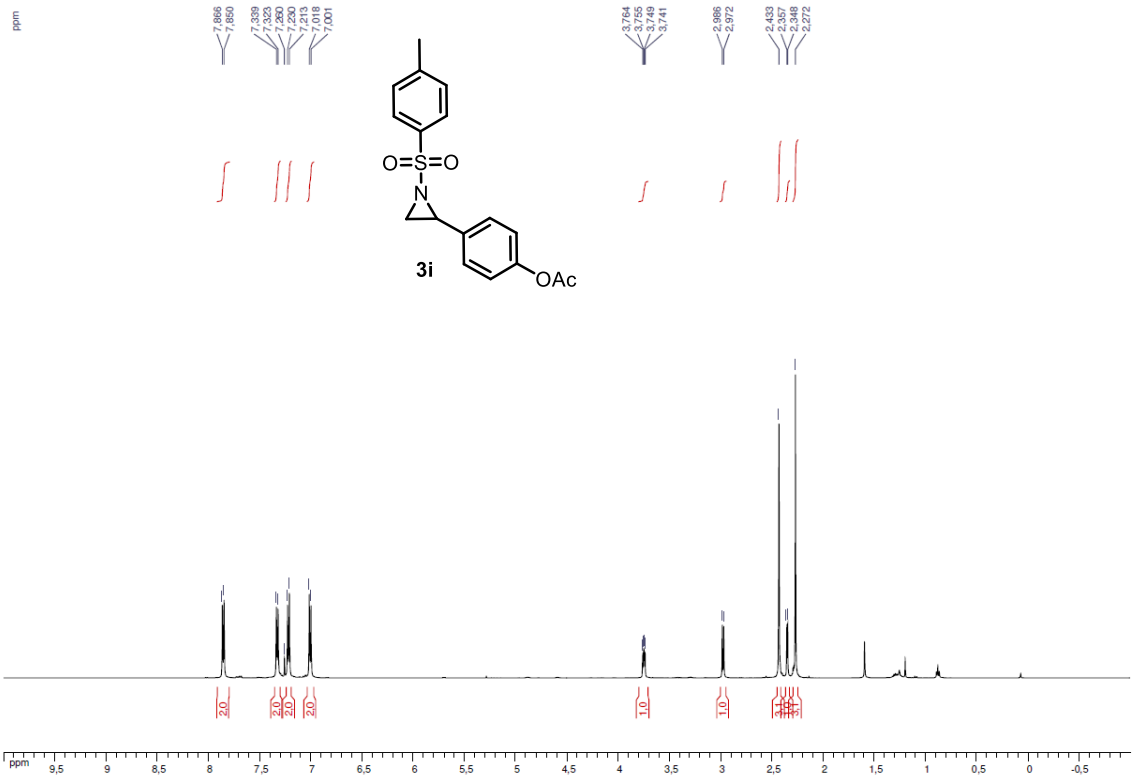
139,371
134,872
131,059
130,800
130,540
130,280
129,991
128,113
127,286
127,066
125,712
125,683
125,134
122,961
120,776
77,413
77,160
76,904
40,288
36,324
21,791
ppm


ppm
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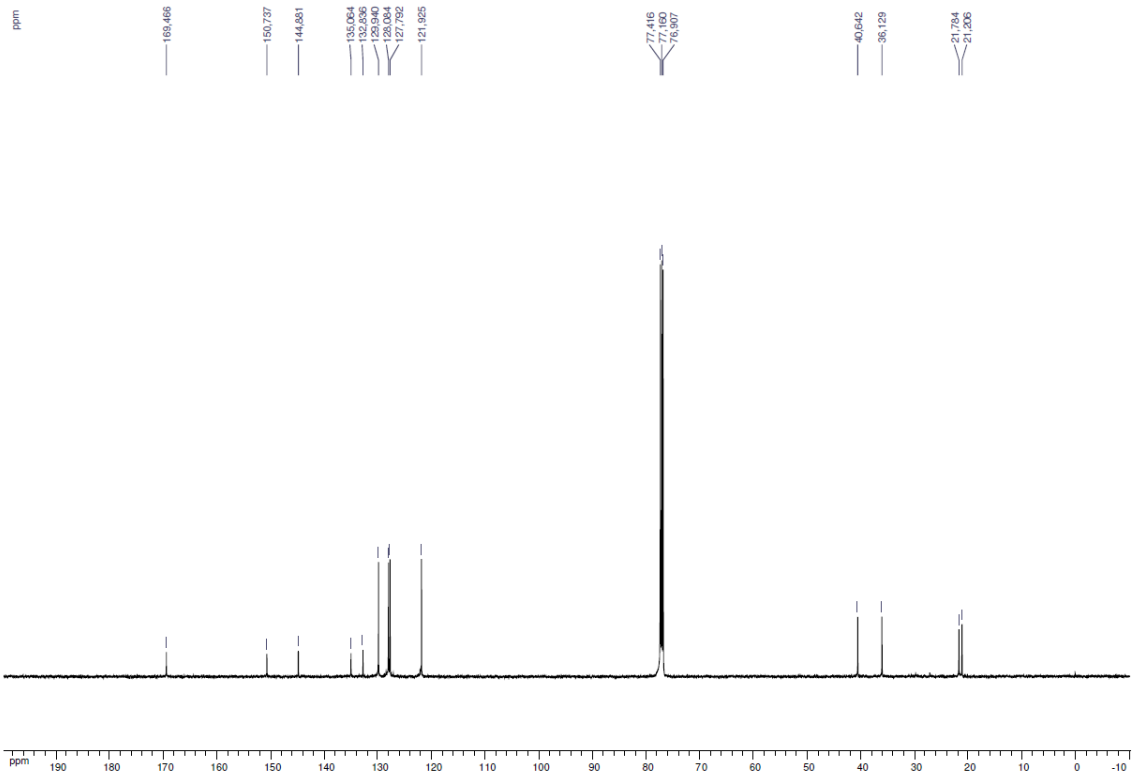
7,323
7,260
7,230
7,213
7,018
7,001
3,764
3,755
3,749
3,741
2,986
2,972
2,433
2,357
2,348
2,272
O=S=O
N
OAc
3i
2,0
2,0
2,0
2,0
1,0
1,0
ppm
9,5
9
8,5
8
7,5
7
6,5
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1
0,5
0
-0,5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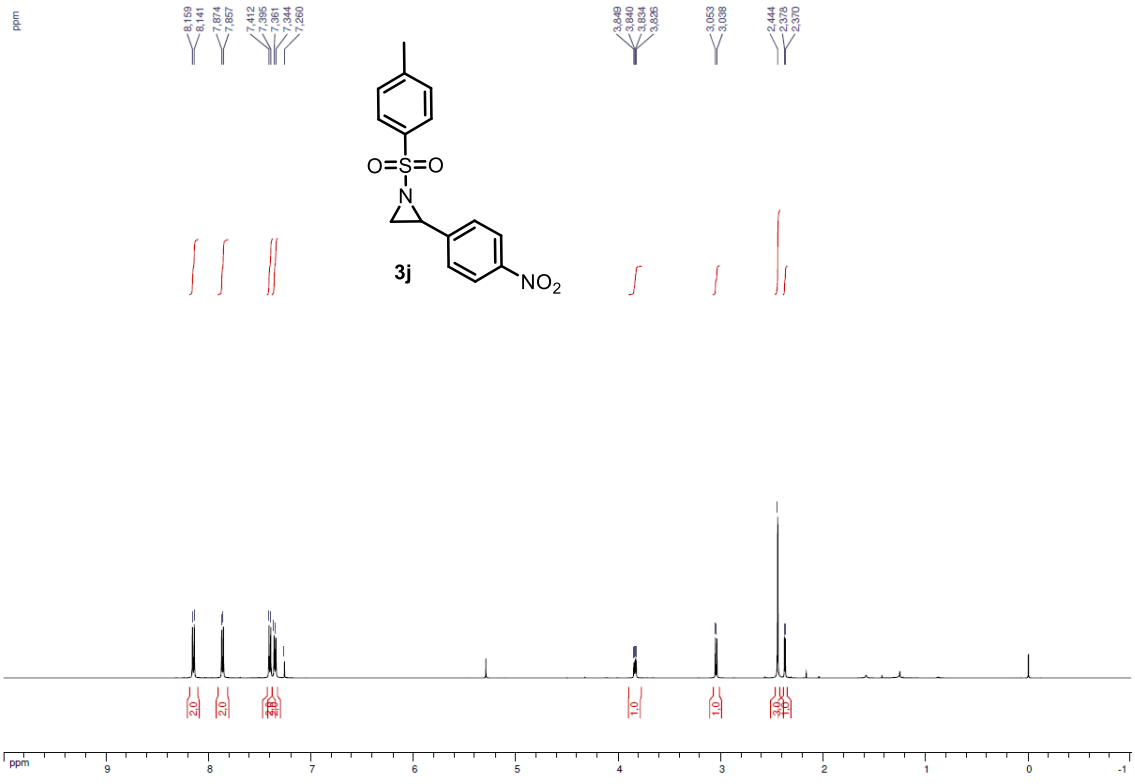
144,881
135,064
132,836
129,940
128,084
127,792
121,925
77,416
77,160
76,907
40,642
36,129
21,784
21,206
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


ppm
8.159
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7.874
7.857
7.412
7.395
7.361
7.344
7.260
3.849
3.840
3.834
3.826
3.053
3.038
2.444
2.378
2.370
O=S=O
N
NO2
3j
2.0
2.0
4.0
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1.0
3.0
1.0
ppm
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8
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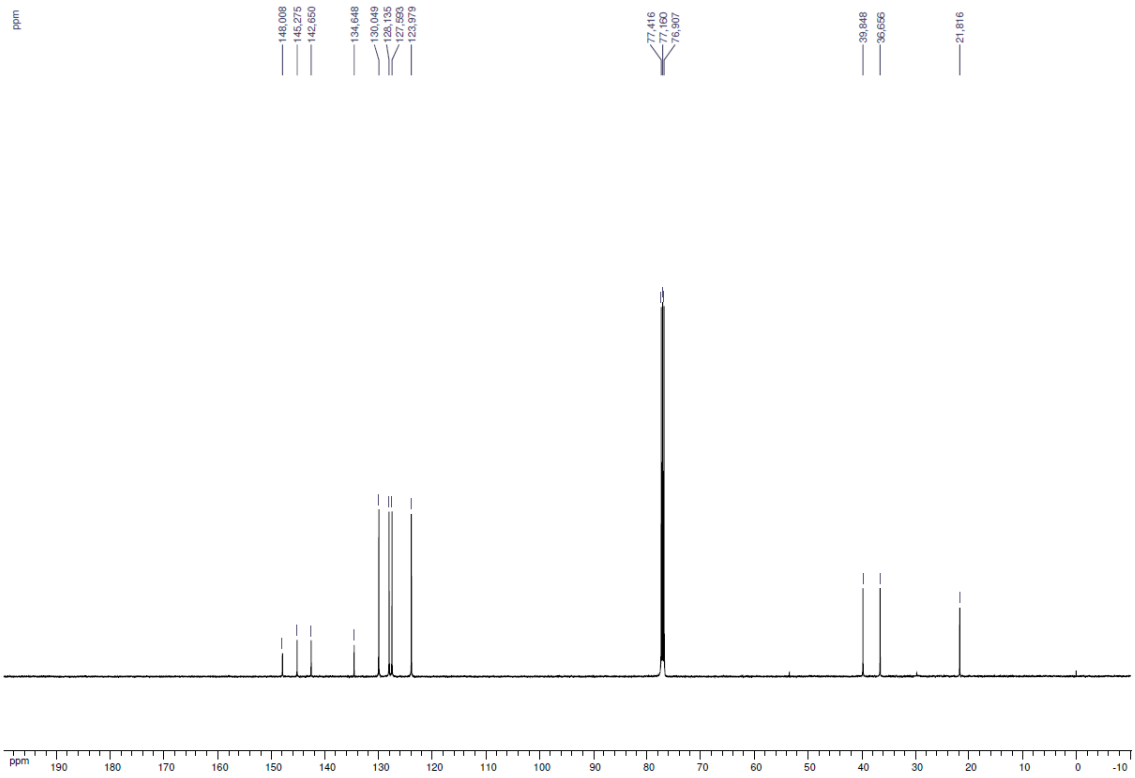
6
5
4
3
2
1
0
-1


ppm
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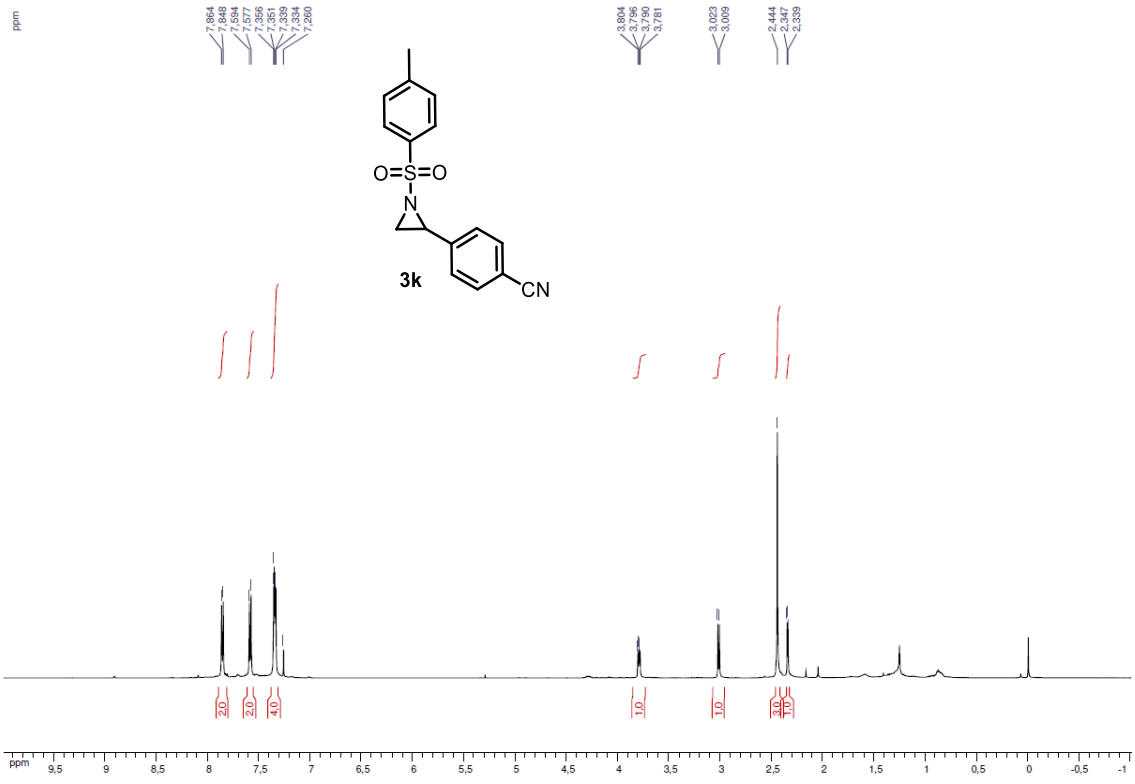
142.650
134.648
130.049
128.135
127.593
123.979
77.416
77.160
76.907
39.848
36.656
21.816
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


ppm
7,864
7,848
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7,577
7,356
7,351
7,339
7,334
7,260
3,804
3,796
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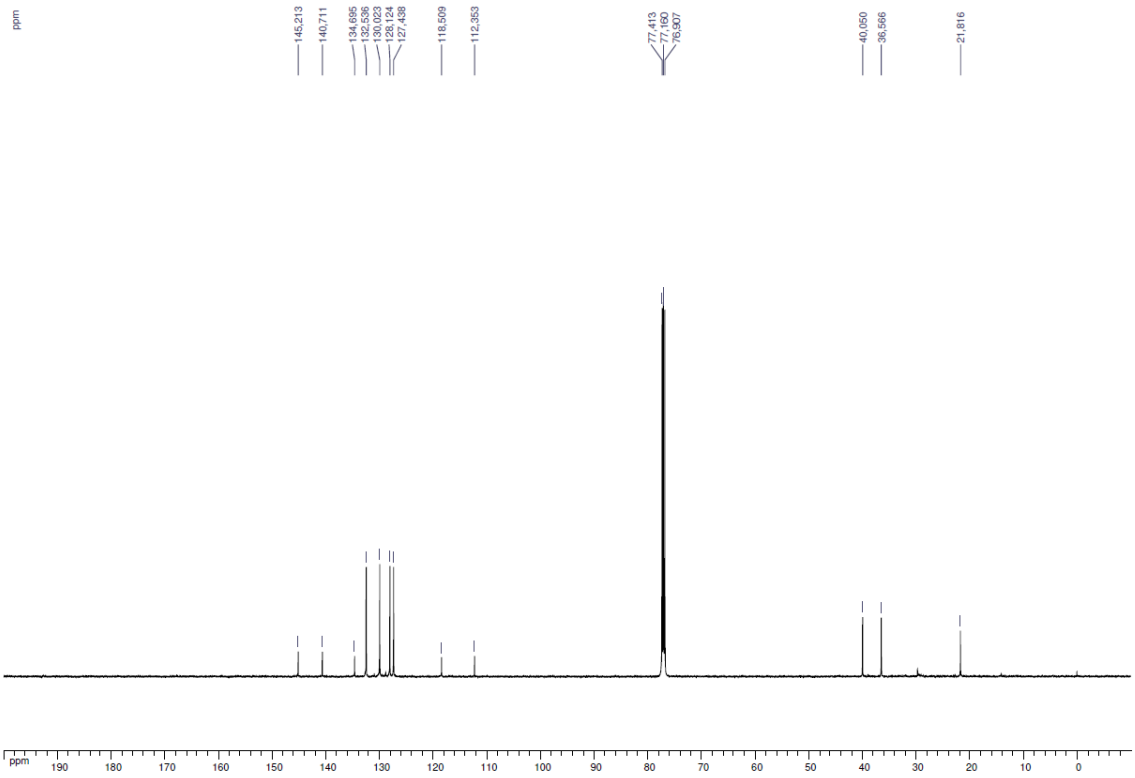
2,347
2,339
O=S=O
N
CN
3k
2,0
2,0
4,0
1,0
1,0
3,0
1,0
ppm
9,5
9
8,5
8
7,5
7
6,5
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1
0,5
0
-0,5
-1


ppm
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128,124
127,438
118,509
112,353
77,413
77,160
76,907
40,050
36,566
21,816
ppm
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180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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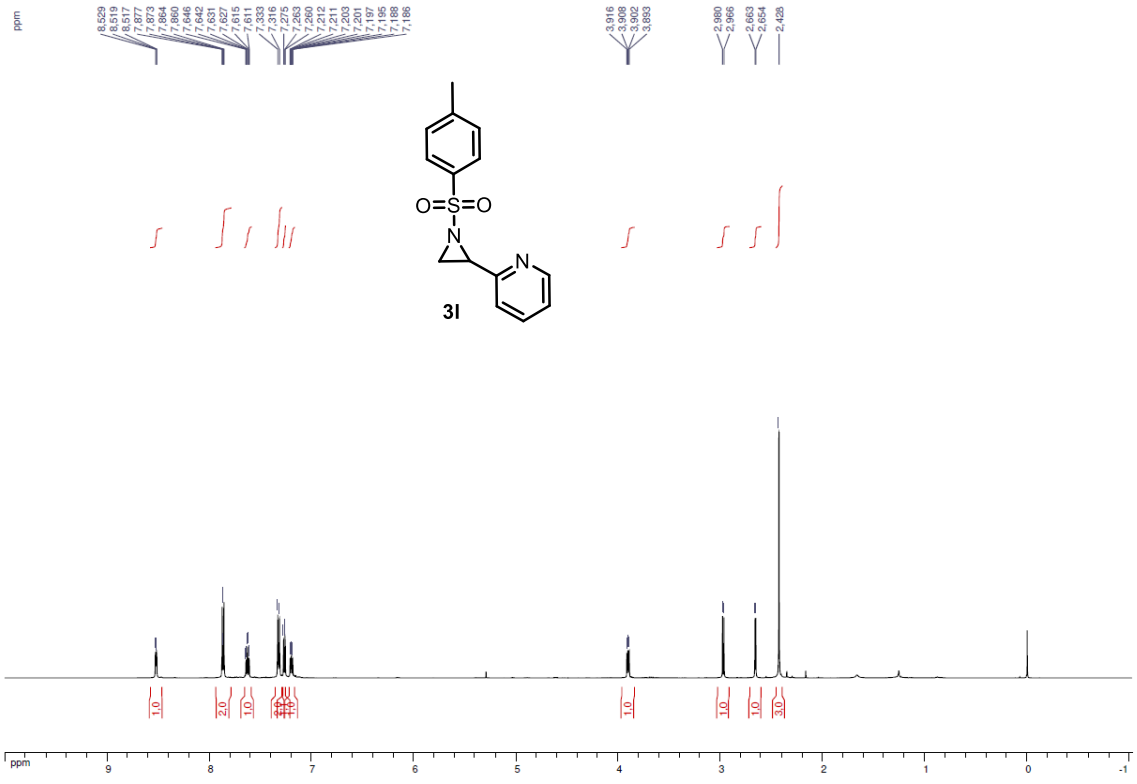
ppm
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8.517
7.877
7.873
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7.646
7.642
7.627
7.621
7.615
7.611
7.333
7.316
7.275
7.263
7.260
7.212
7.211
7.203
7.201
7.197
7.195
7.188
7.186
3.916
3.908
3.902
3.893
2.980
2.966
2.663
2.654
2.425
O=S=O
N
N
3l
1.0
2.0
1.0
1.0
1.0
1.0
1.0
3.0
ppm
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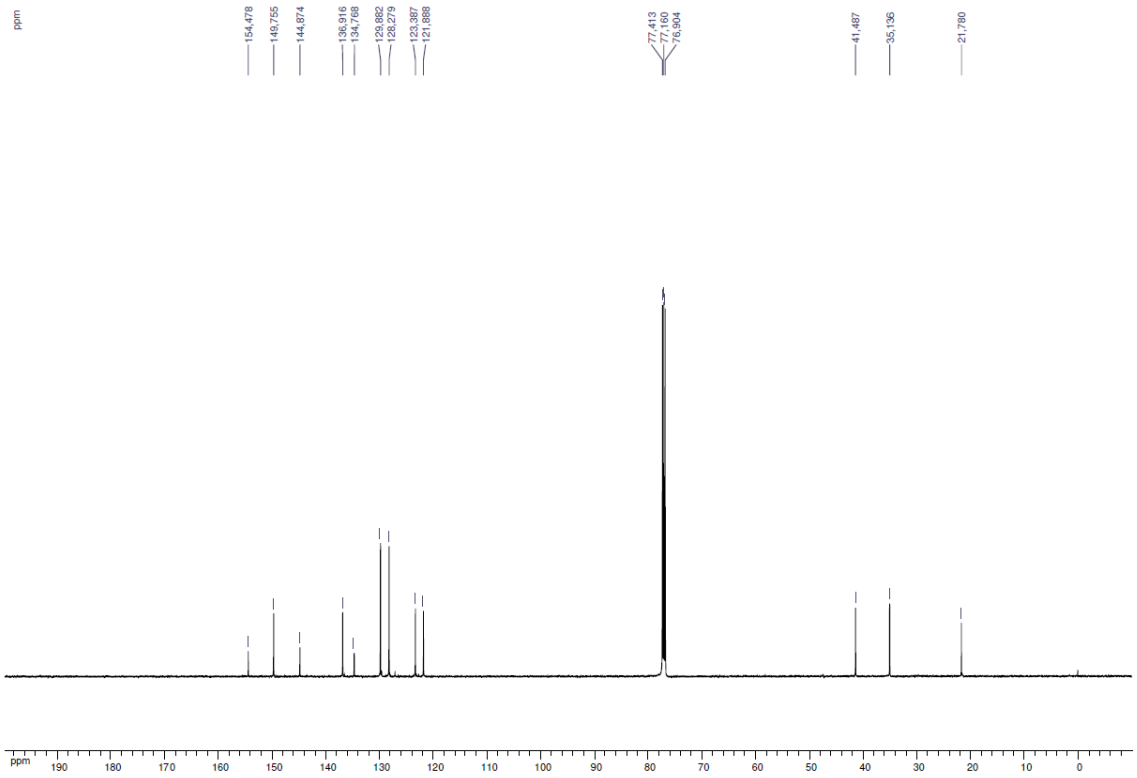
8
7
6
5
4
3
2
1
0
-1


ppm
154.478
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144.874
136.916
134.768
129.882
128.279
123.387
121.888
77.413
77.160
76.904
41.487
35.136
21.780
ppm
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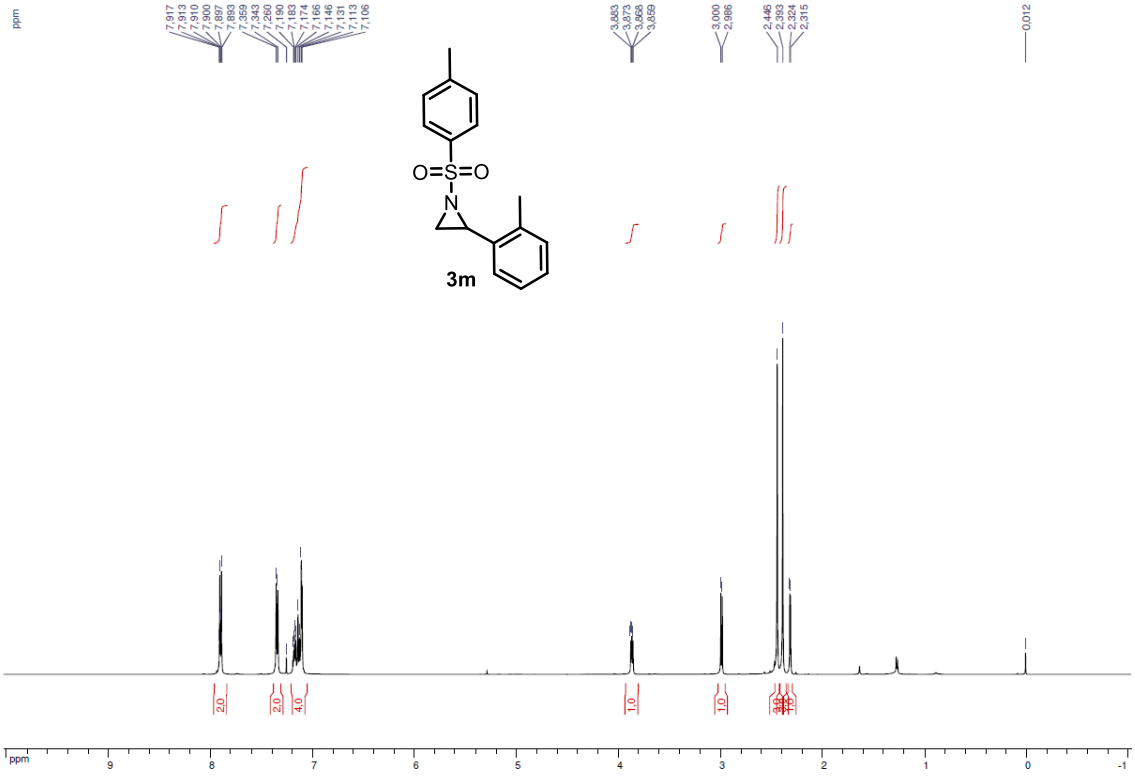
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


ppm
7,917
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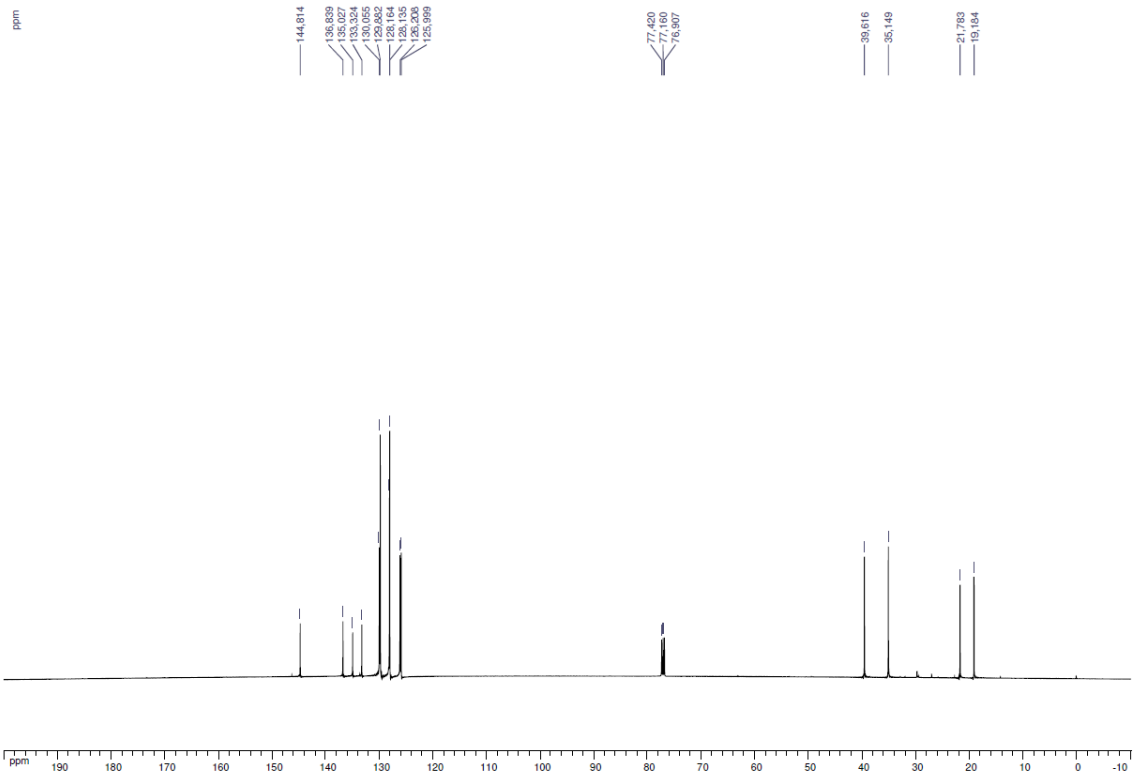
7,910
7,900
7,897
7,893
7,359
7,343
7,260
7,189
7,183
7,174
7,166
7,146
7,131
7,113
7,106
3,983
3,973
3,968
3,959
3,000
2,986
2,446
2,393
2,324
2,315
0,012
O=S=O
N
3m
2,0
2,0
4,0
1,0
1,0
ppm
9
8
7
6
5
4
3
2
1
0
-1


ppm
144,814
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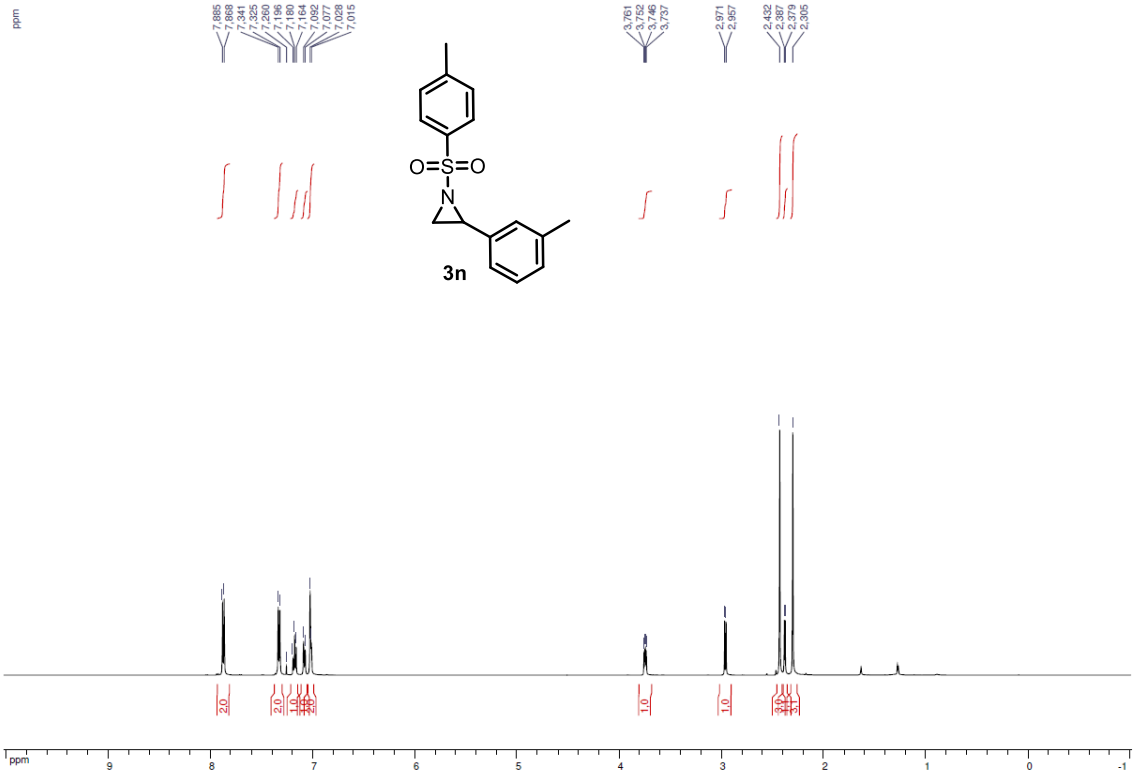
135,027
133,324
130,055
129,843
128,164
128,135
126,206
125,999
77,420
77,160
76,907
39,616
35,149
21,783
19,184
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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7.269
7.196
7.180
7.164
7.092
7.077
7.028
7.015
3.761
3.752
3.746
3.737
2.971
2.957
2.432
2.387
2.379
2.305
3n

ppm
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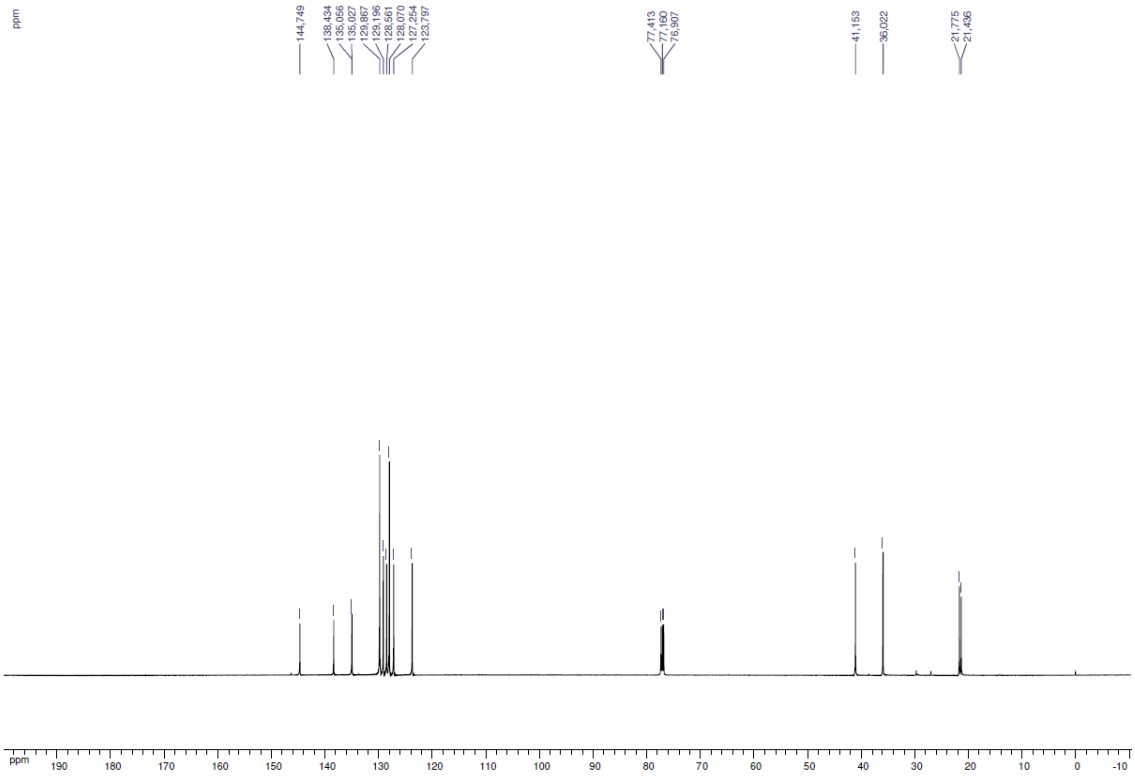
2.0
1.0
1.0
3.0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144.749
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135.056
135.027
129.957
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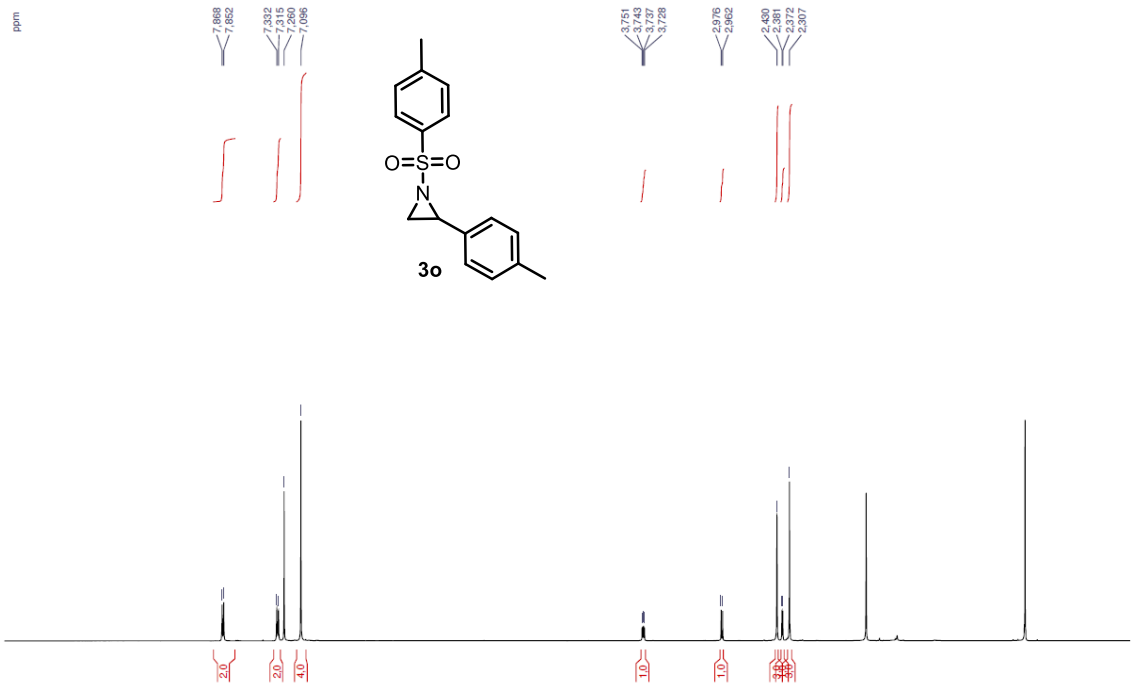
128.561
128.070
127.254
123.797
77.413
77.160
76.907
41.153
36.022
21.775
21.436


ppm
7.868
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7.332
7.315
7.260
7.096
3.751
3.743
3.737
3.728
2.976
2.962
2.430
2.381
2.372
2.307
O=S=O
N
3o
2.0
2.0
4.0
1.0
1.0
3.0
3.0
3.0
ppm
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6
5
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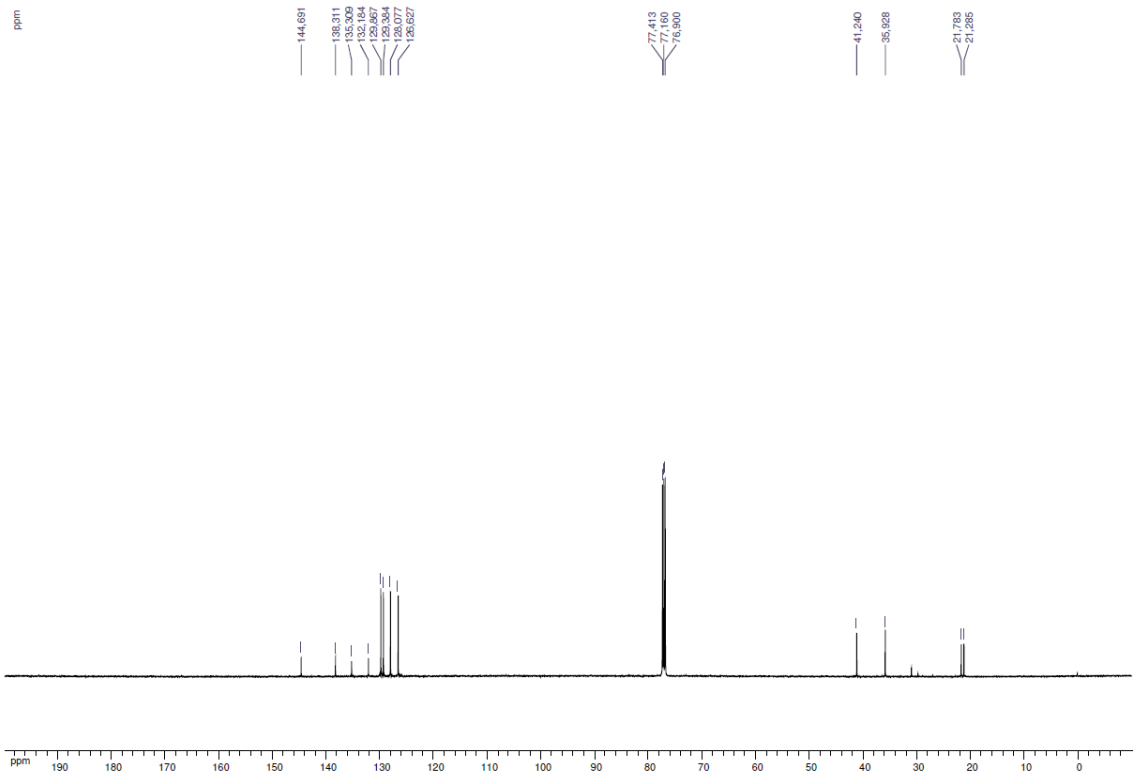
2
1
0
-1


ppm
144.691
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132.184
129.867
129.394
128.077
126.627
77.413
77.160
76.900
41.240
35.928
21.783
21.285
ppm
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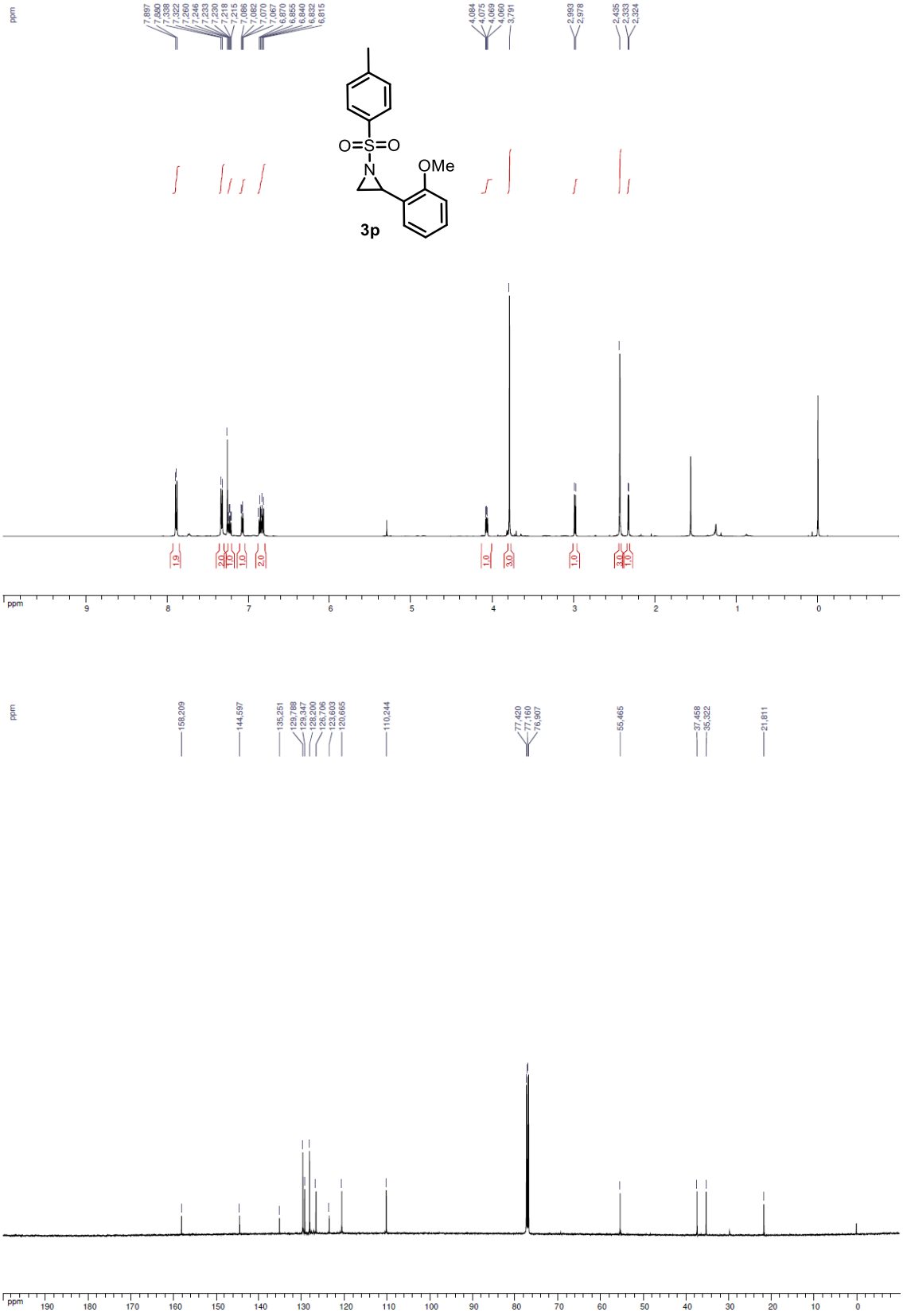
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


ppm
7,897
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7,322
7,260
7,246
7,233
7,230
7,218
7,215
7,088
7,082
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6,840
6,832
6,815
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4,075
4,069
4,060
3,791
2,993
2,978
2,435
2,333
2,324
O=S=O
N
OMe
3p
1,9
2,0
1,0
1,0
2,0
1,0
3,0
1,0
3,0
1,0
ppm
9
8
7
6
5
4
3
2
1
0
ppm
158,209
144,597
135,251
129,788
129,347
128,200
126,705
123,603
120,665
110,244
77,420
77,160
76,907
55,465
37,458
35,322
21,811
ppm
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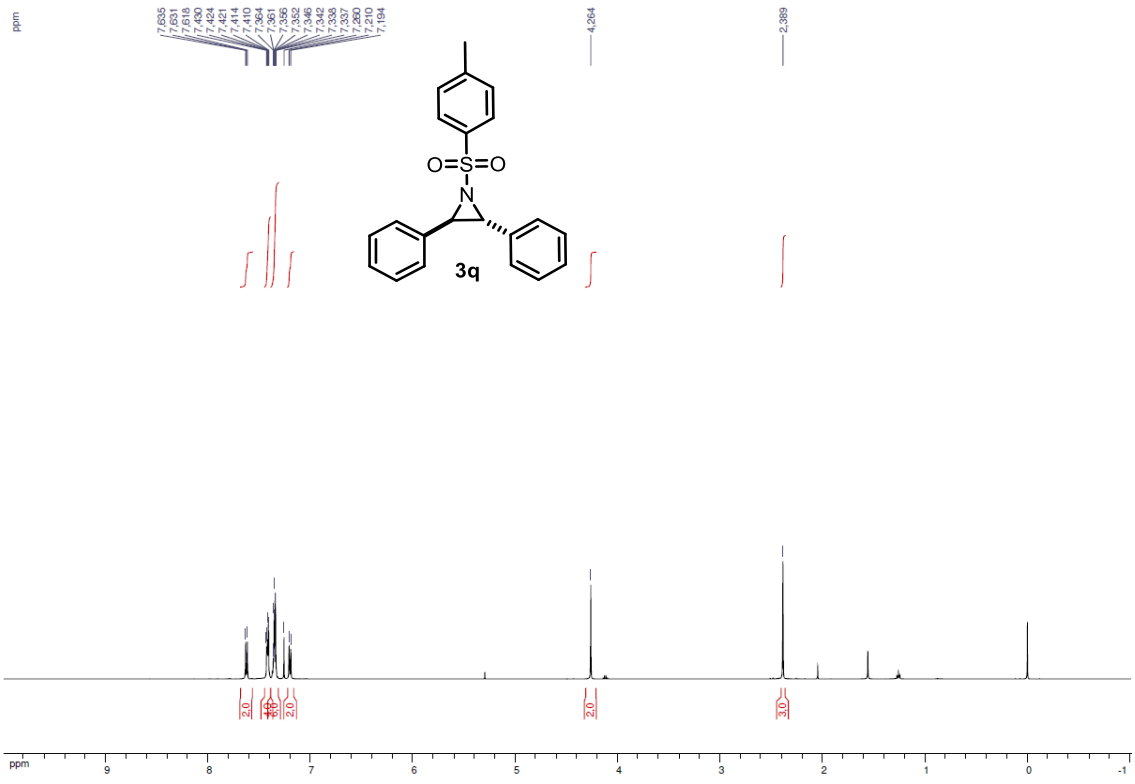
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


ppm
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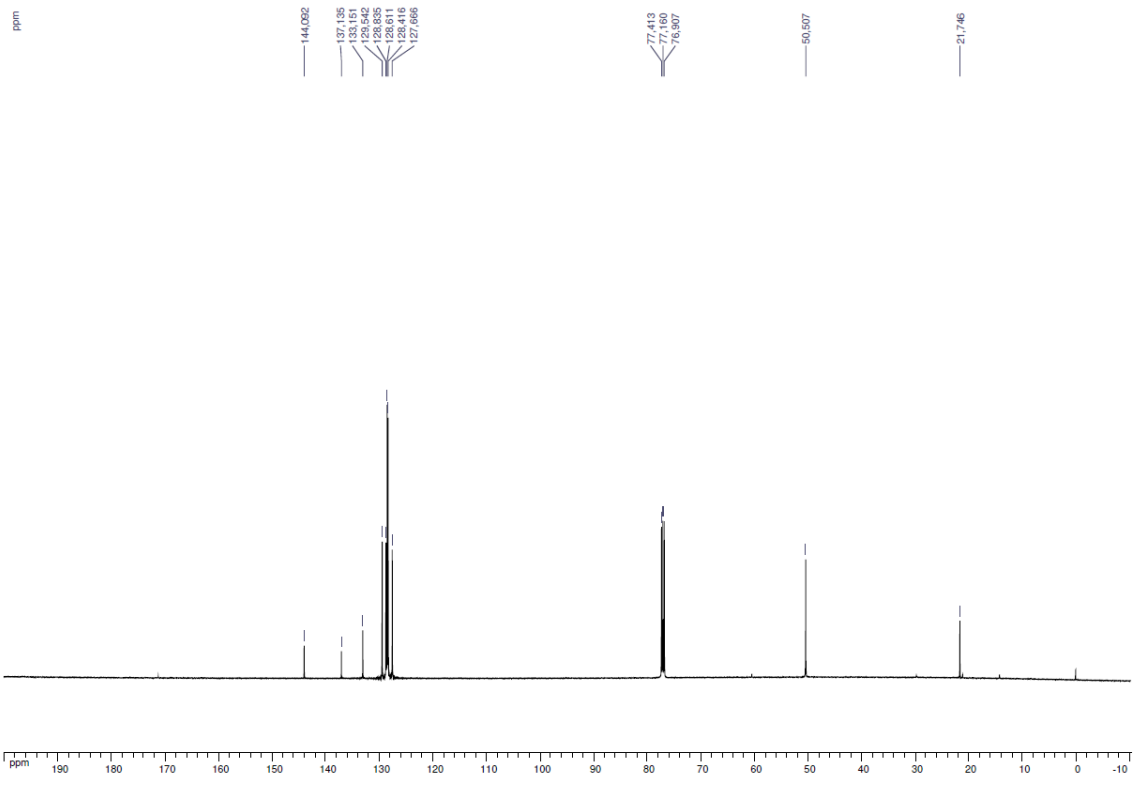
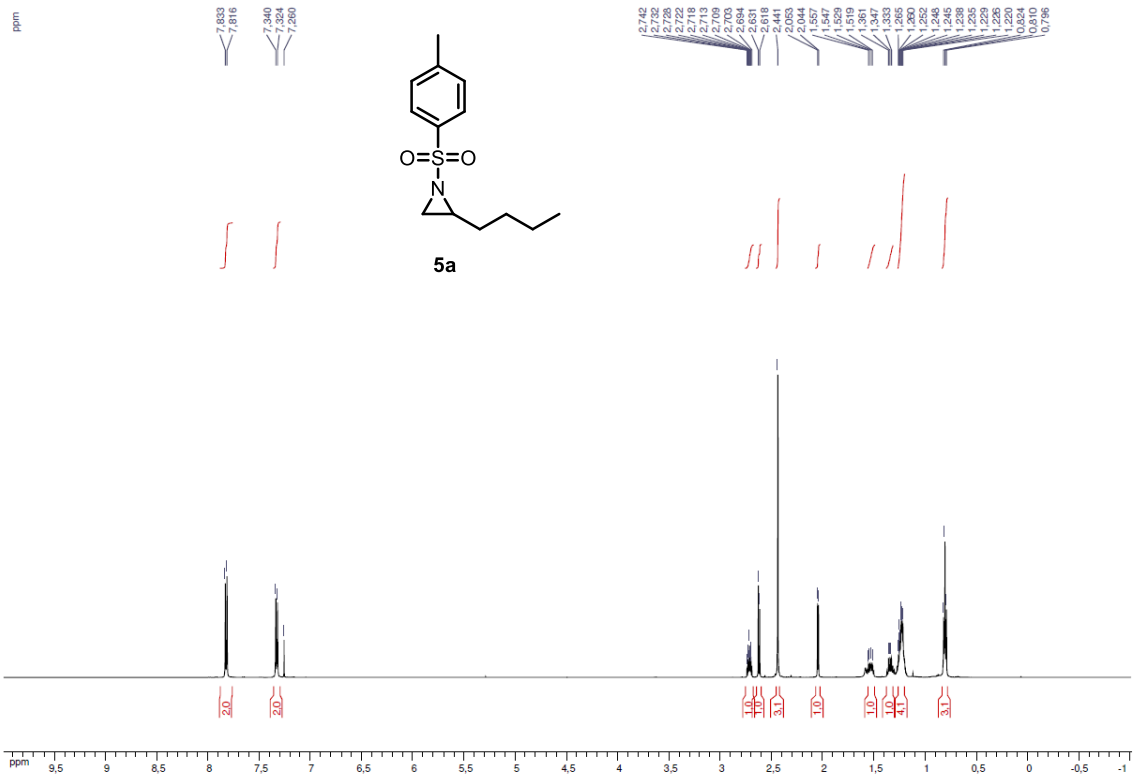
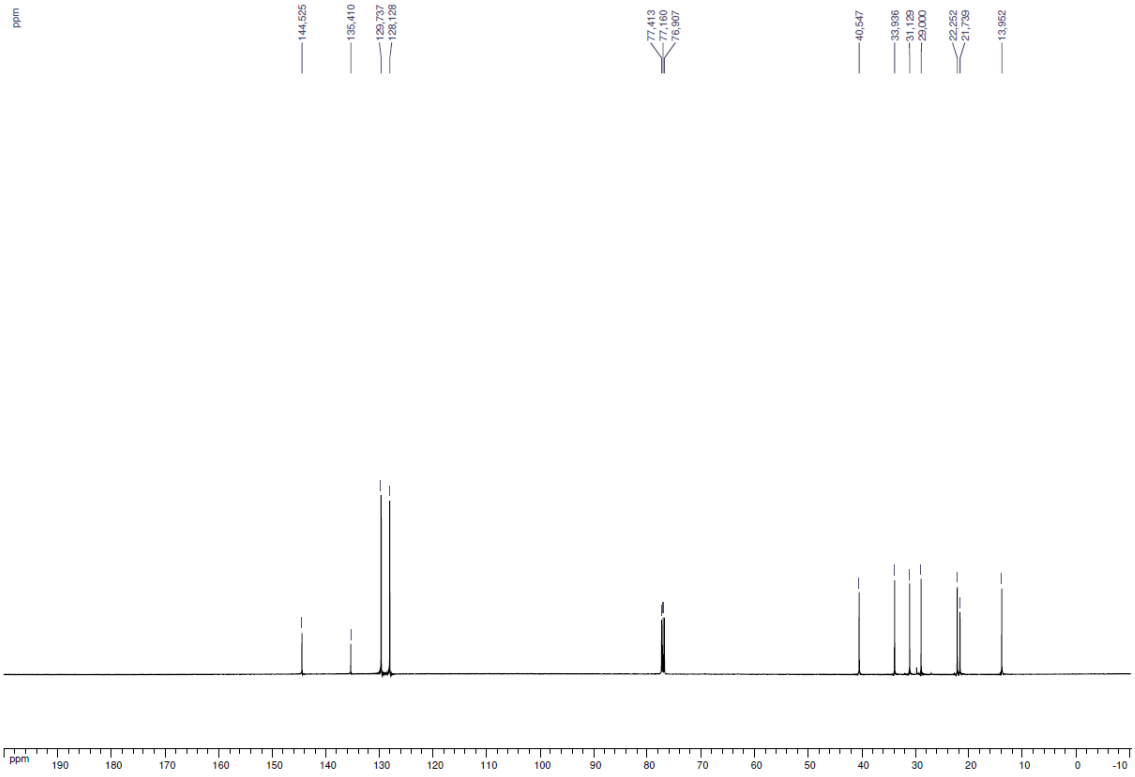
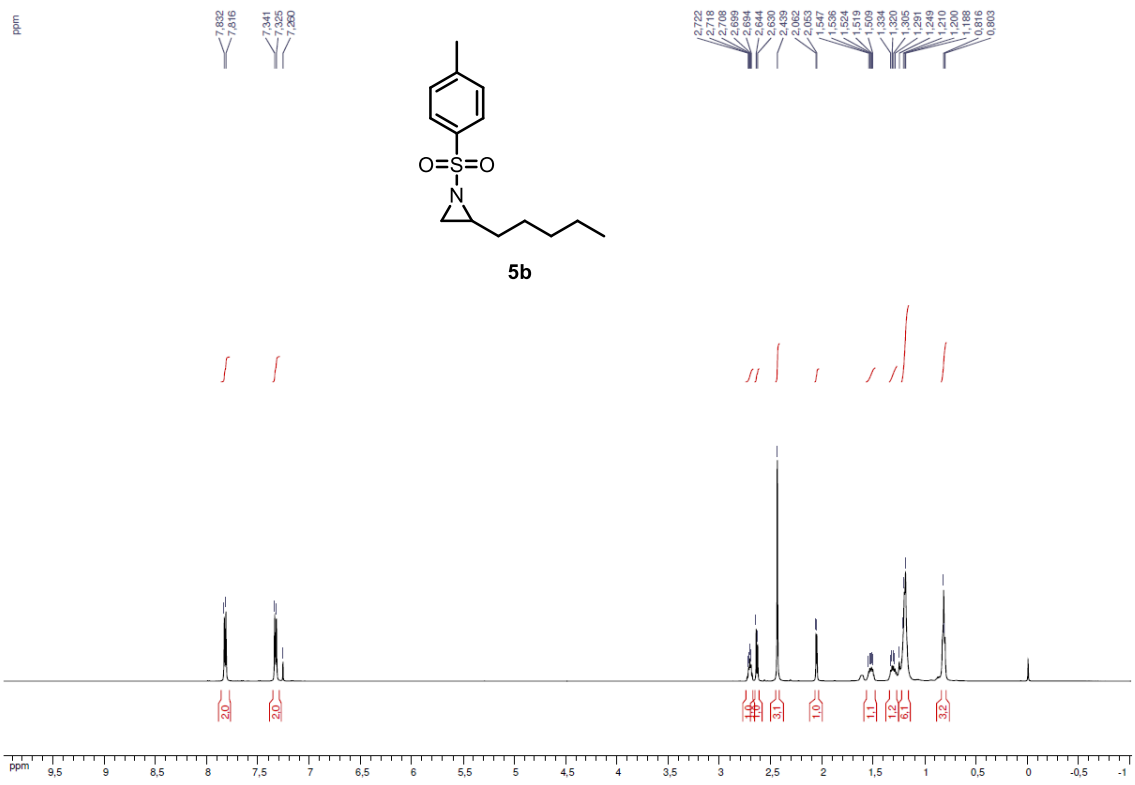
7.631
7.618
7.430
7.424
7.421
7.414
7.410
7.364
7.361
7.356
7.332
7.346
7.342
7.338
7.337
7.290
7.210
7.194
4.264
2.389
O=S=O
N
3q
2.0
4.6
2.0
2.0
3.0
ppm
9
8
7
6
5
4
3
2
1
0
-1

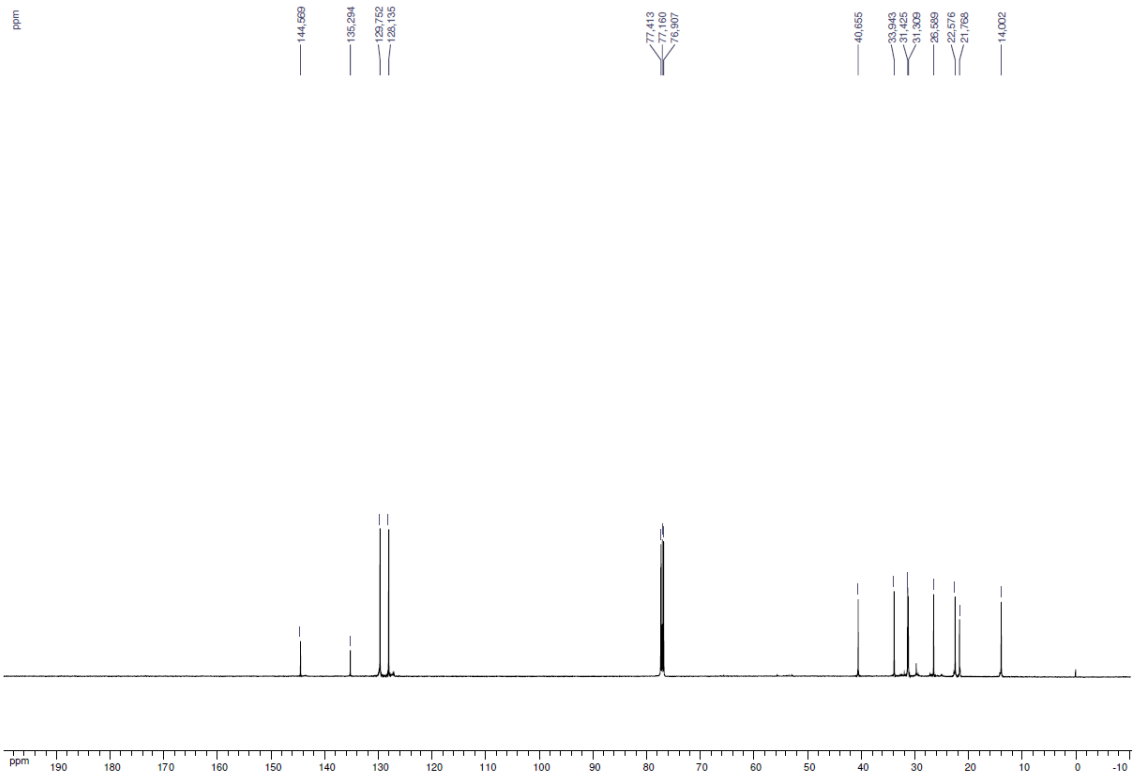

ppm
144.092
137.135
133.151
129.642
129.365
128.611
128.416
127.666
77.413
77.160
76.907
50.507
21.746
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

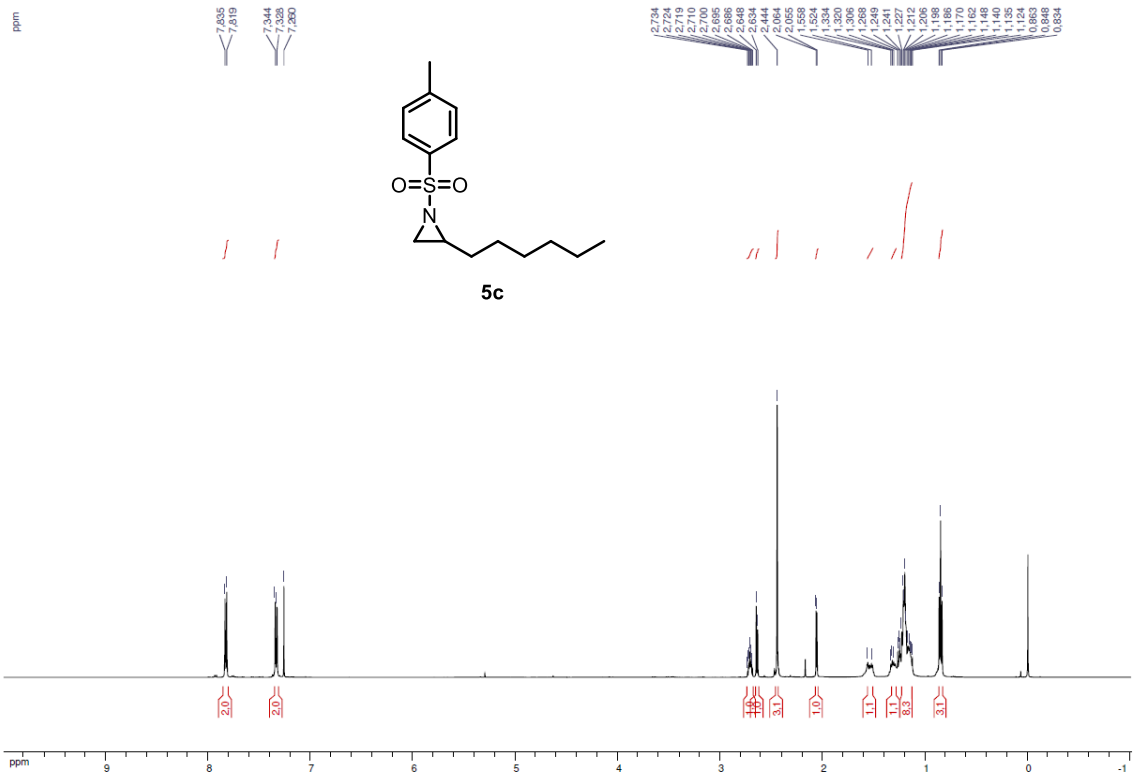

ppm
7,833
7,816
7,340
7,324
7,260
2,742
2,732
2,728
2,722
2,718
2,713
2,709
2,703
2,694
2,631
2,618
2,441
2,053
2,044
1,557
1,547
1,529
1,519
1,361
1,347
1,333
1,265
1,260
1,252
1,245
1,238
1,235
1,229
1,226
1,220
1,044
0,810
0,796
O=S=O
N
5a
2,0
2,0
1,0
1,0
3,1
1,0
1,0
1,0
4,1
3,1
ppm
9,5
9
8,5
8
7,5
7
6,5
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1
0,5
0
-0,5
-1

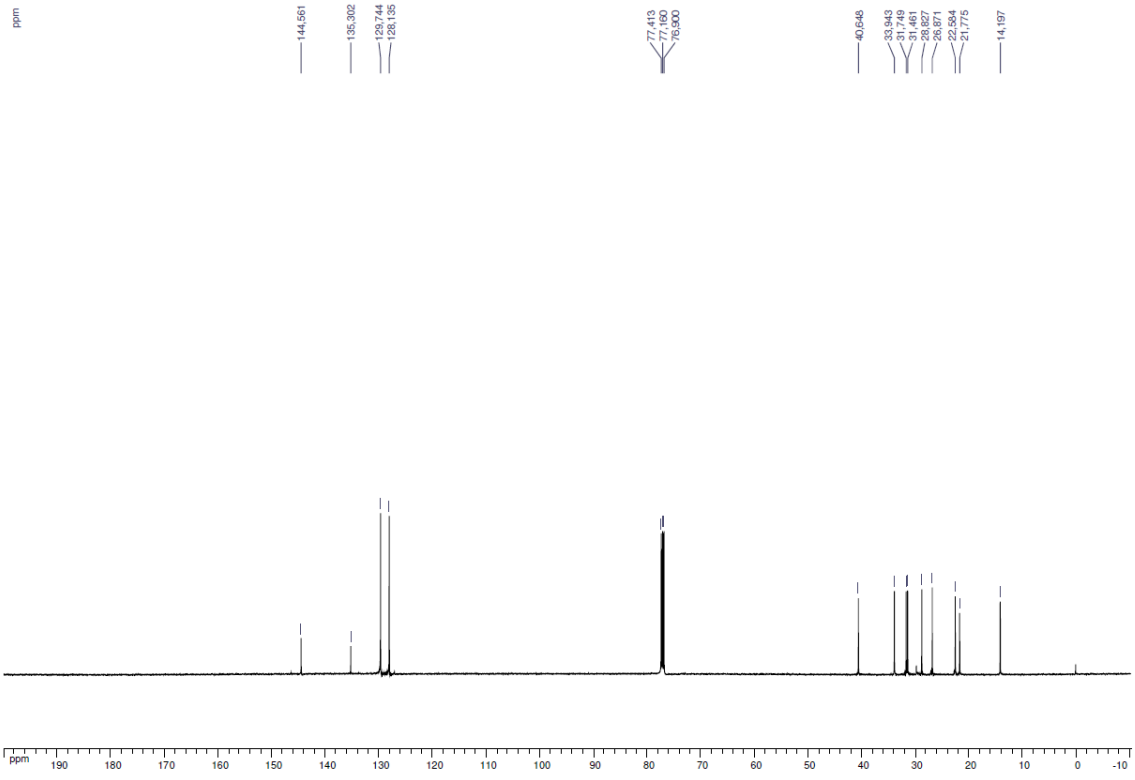

ppm
144,525
135,410
129,737
128,128
77,413
77,160
76,907
40,547
33,936
31,129
29,000
22,252
21,739
13,952
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

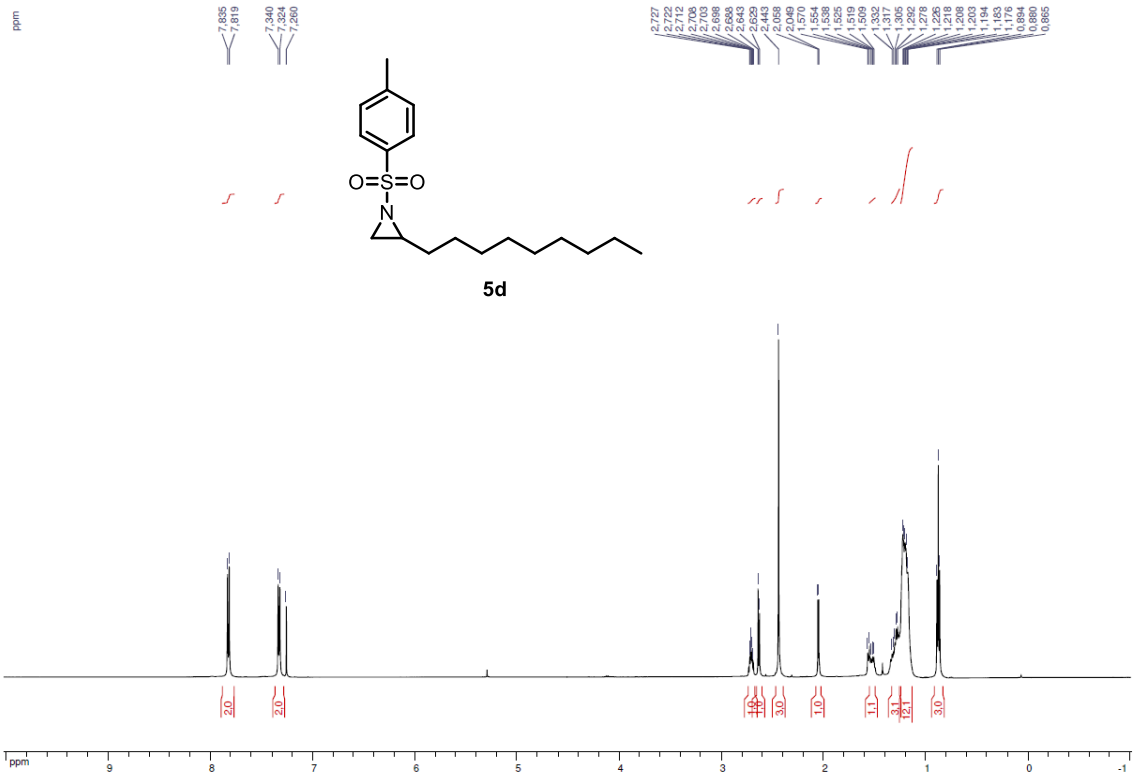

ppm
7,832
7,816
7,341
7,325
7,260
2,722
2,718
2,708
2,699
2,694
2,644
2,630
2,489
2,062
2,053
1,547
1,536
1,524
1,519
1,509
1,334
1,320
1,305
1,291
1,249
1,210
1,200
1,188
0,815
0,803
O=S=O
N
2,0
2,0
1,0
3,1
1,0
1,1
1,2
6,1
3,2
ppm
9,5
9
8,5
8
7,5
7
6,5
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1
0,5
0
-0,5
-1

5b

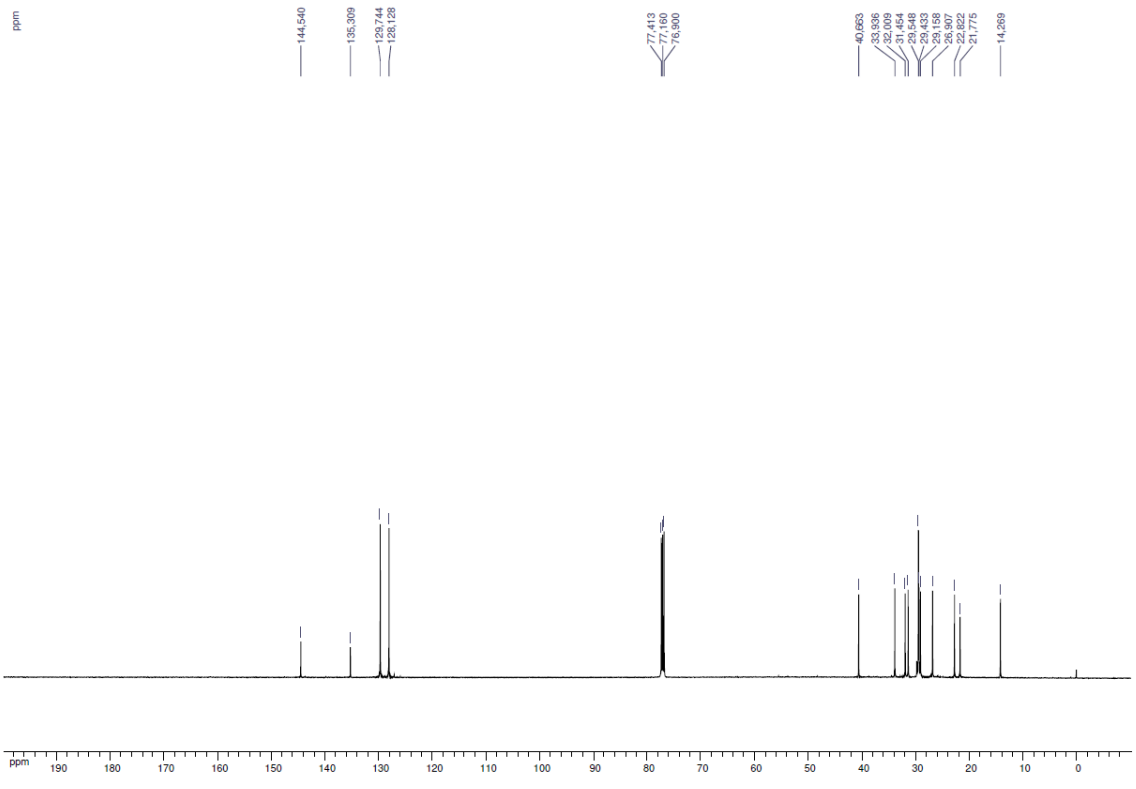

ppm
144,569
135,294
129,752
128,135
77,413
77,160
76,907
40,655
33,943
31,425
31,309
26,599
22,576
21,768
14,002
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

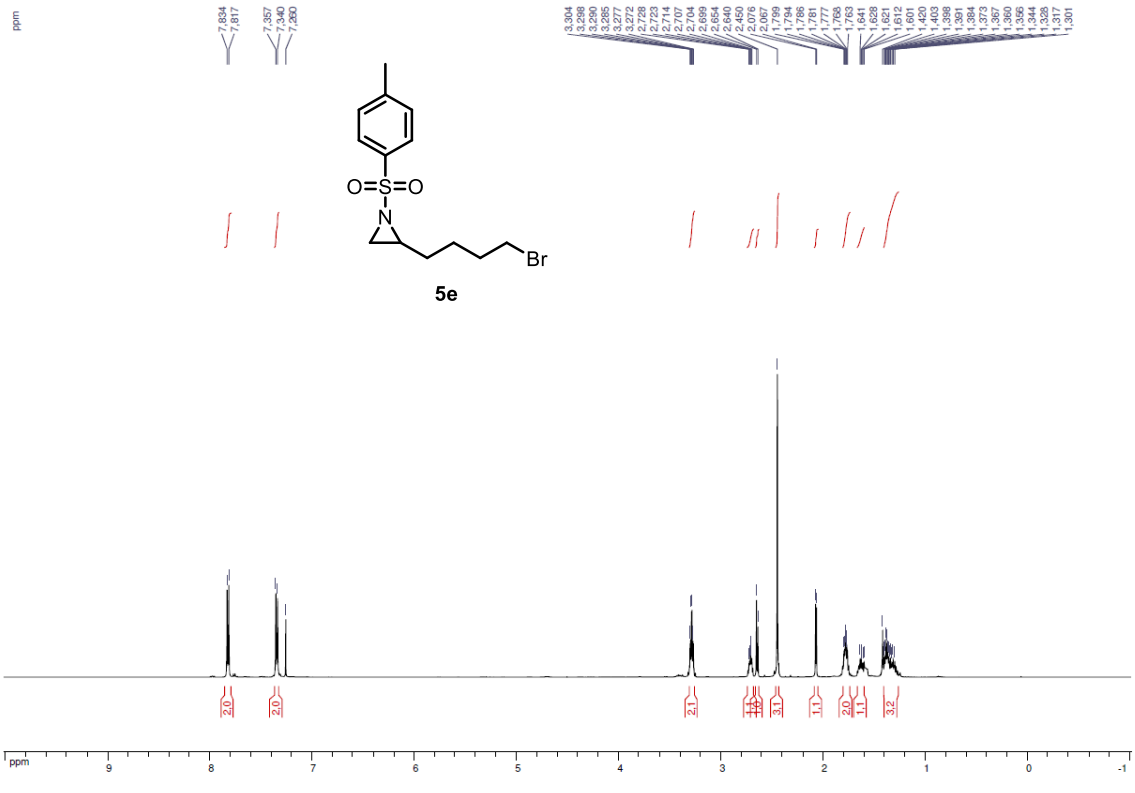

ppm
7,835
7,819
7,344
7,338
7,300
2,734
2,724
2,719
2,710
2,700
2,695
2,688
2,648
2,634
2,444
2,064
2,055
1,558
1,524
1,334
1,320
1,306
1,288
1,249
1,241
1,227
1,212
1,206
1,198
1,186
1,170
1,162
1,148
1,140
1,135
1,124
0,863
0,848
0,834
O=S=O
N
5c
2,0
2,0
1,0
1,1
1,1
8,3
3,1
ppm
9
8
7
6
5
4
3
2
1
0
-1

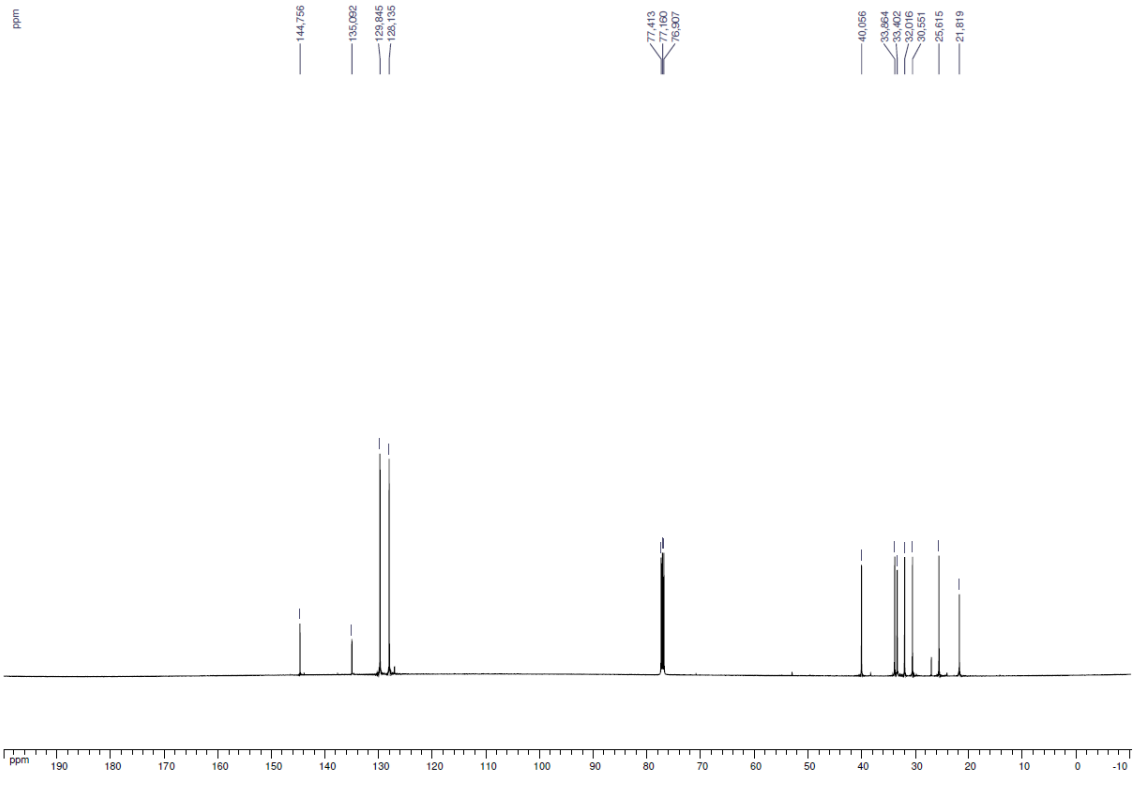

ppm
144,561
135,302
129,744
128,135
77,413
77,160
76,900
40,646
33,943
31,749
31,461
28,827
28,671
22,394
21,775
14,197
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

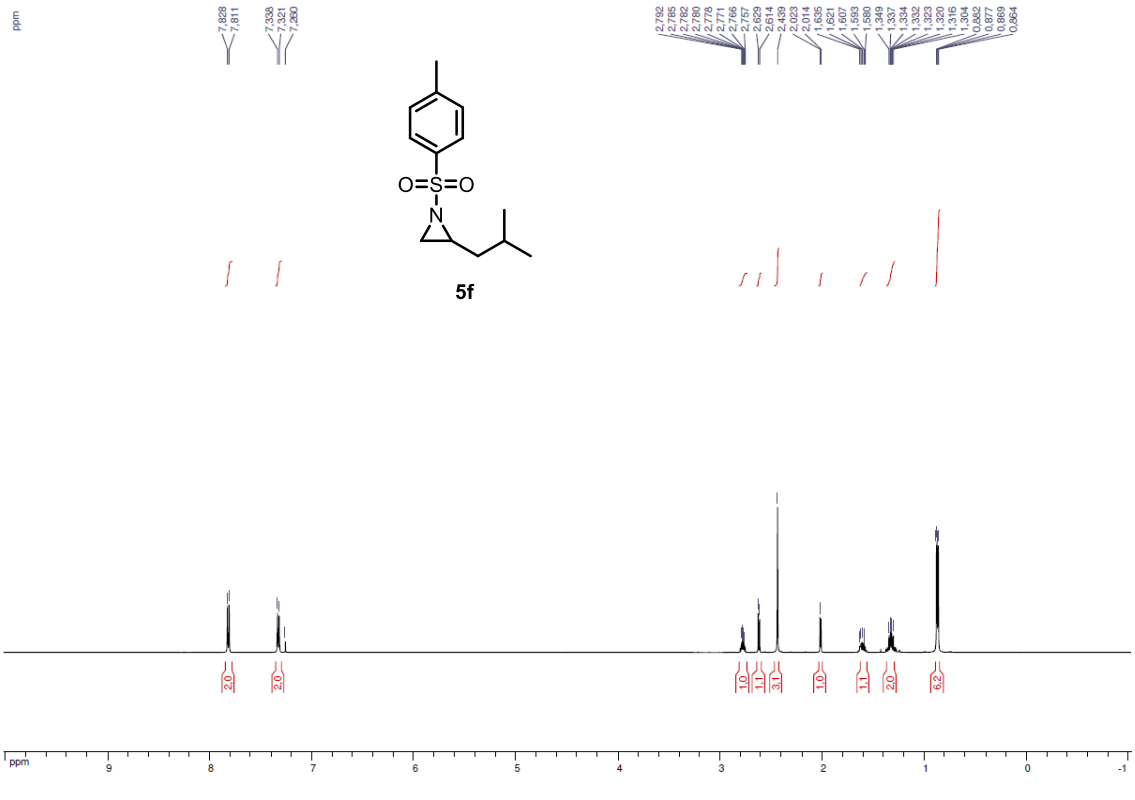

ppm
7.835
7.819
7.340
7.324
7.260
2.727
2.722
2.712
2.706
2.703
2.698
2.688
2.643
2.629
2.443
2.058
2.049
1.570
1.554
1.538
1.525
1.519
1.509
1.332
1.317
1.305
1.292
1.278
1.226
1.218
1.208
1.203
1.194
1.183
1.176
0.894
0.880
0.865
O=S=O
N
2.0
2.0
1.0
3.0
1.0
1.1
3.1
12.1
3.0
ppm
9
8
7
6
5
4
3
2
1
0
-1

5d

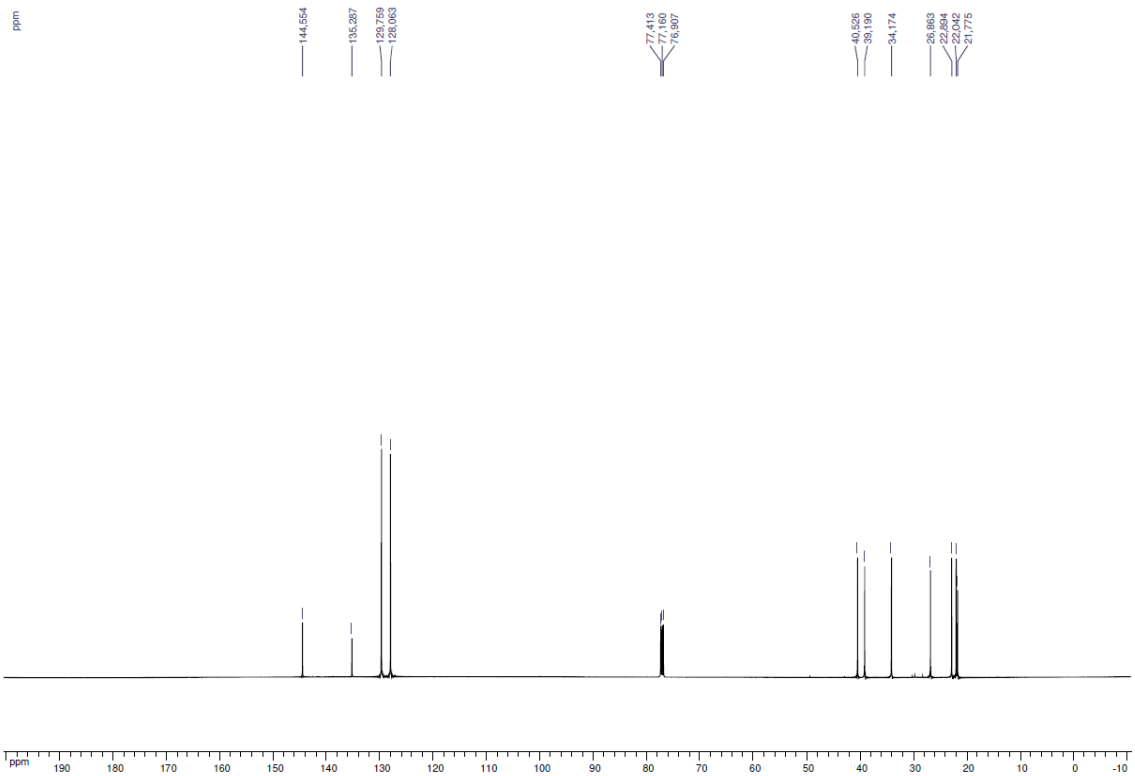

ppm
144.540
135.309
129.744
126.128
77.413
77.160
76.900
40.663
33.936
32.009
31.454
29.548
29.453
29.158
26.907
22.822
21.775
14.269
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

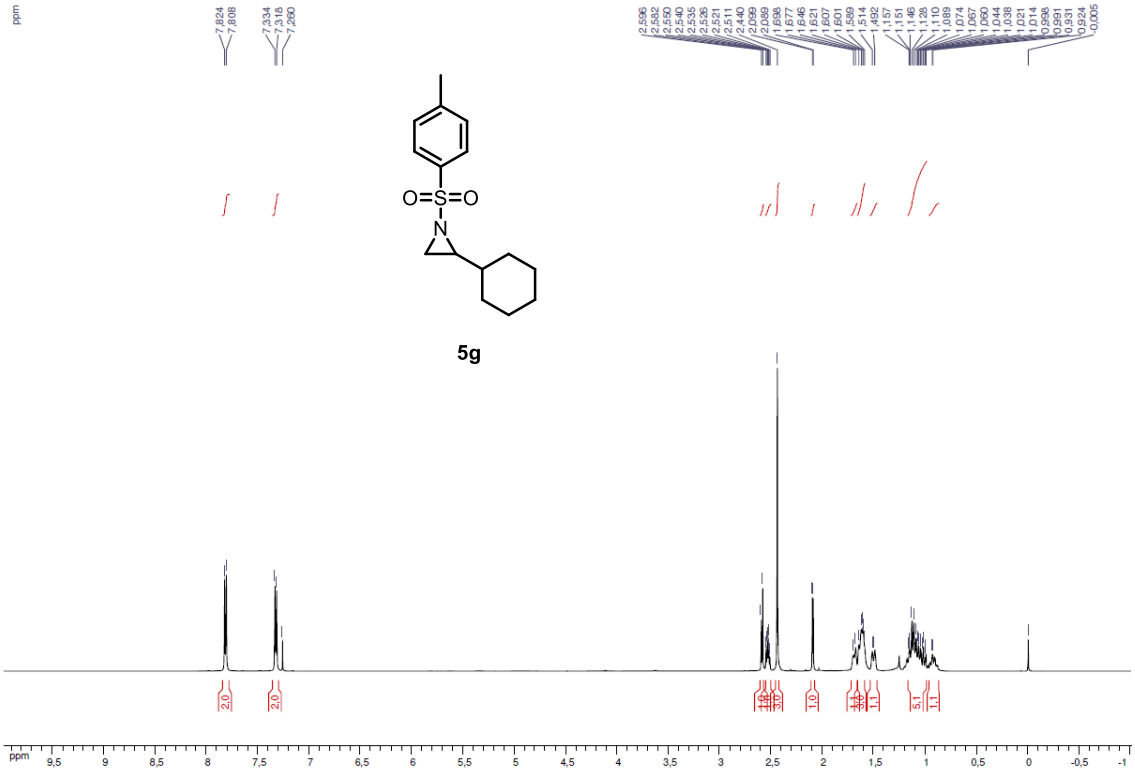

ppm
7.834
7.817
7.357
7.340
7.260
3.304
3.298
3.290
3.285
3.277
3.272
2.728
2.723
2.714
2.707
2.704
2.699
2.654
2.646
2.450
2.076
2.067
1.799
1.794
1.786
1.781
1.777
1.768
1.763
1.641
1.628
1.621
1.612
1.601
1.420
1.403
1.398
1.391
1.384
1.373
1.367
1.360
1.356
1.344
1.328
1.317
1.301
O=S=O
N
Br
5e
2.0
2.0
2.1
1.0
3.1
1.1
2.0
1.1
3.2
ppm
9
8
7
6
5
4
3
2
1
0
-1


ppm
144.756
135.092
129.845
128.155
77.413
77.160
76.907
40.056
33.964
33.402
32.705
30.551
25.615
21.819
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

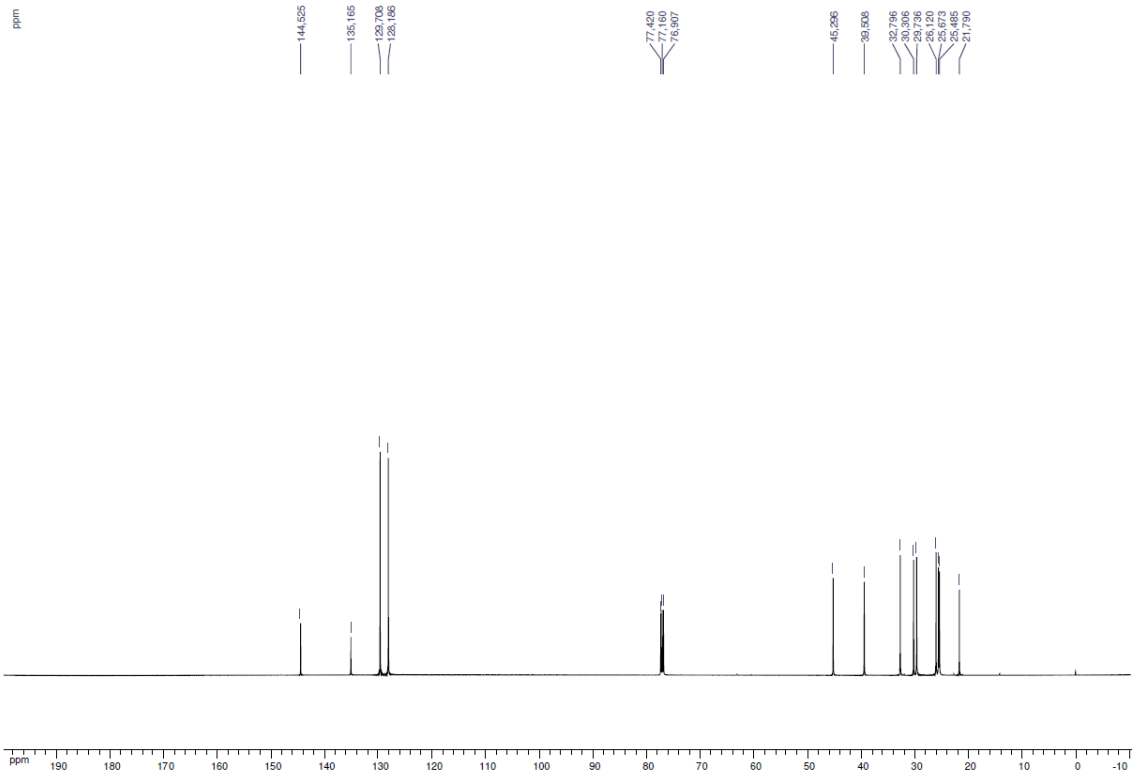

ppm
7.828
7.811
7.338
7.321
7.260
2.792
2.785
2.778
2.780
2.778
2.771
2.766
2.757
2.629
2.614
2.439
2.023
2.014
1.635
1.621
1.607
1.593
1.589
1.349
1.337
1.334
1.332
1.323
1.320
1.316
1.304
0.882
0.877
0.869
0.864
O=S=O
N
2.0
2.0
1.0
1.1
3.1
1.0
1.1
2.0
6.2
ppm
9
8
7
6
5
4
3
2
1
0
-1

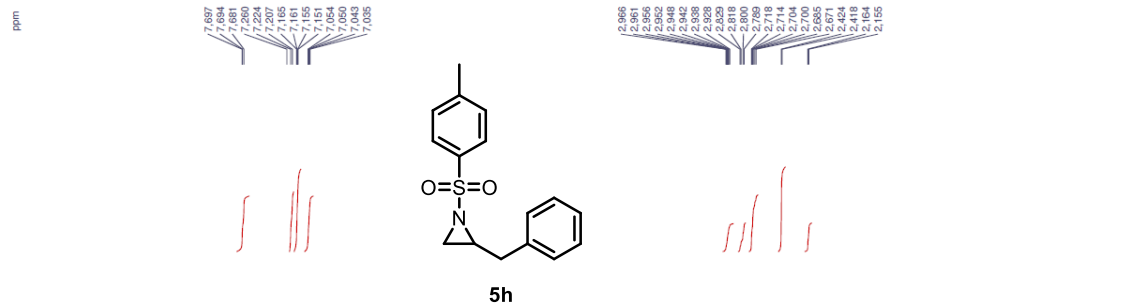
5f


ppm
144.554
135.287
129.759
128.063
77.413
77.160
76.907
40.526
39.190
34.174
26.863
22.894
22.042
21.775
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

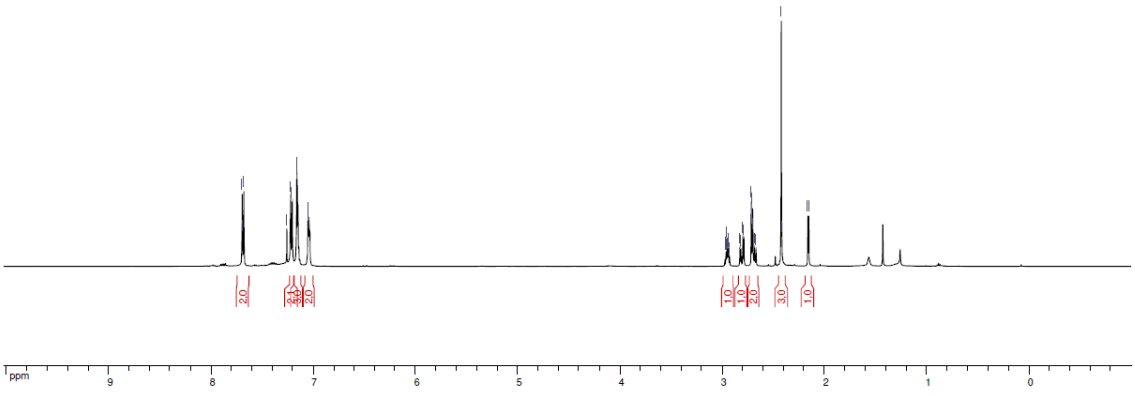

ppm
7,824
7,808
7,334
7,318
7,260
2,596
2,582
2,550
2,540
2,535
2,526
2,521
2,511
2,440
2,099
2,089
1,696
1,677
1,646
1,621
1,607
1,601
1,589
1,514
1,492
1,157
1,151
1,146
1,128
1,110
1,089
1,074
1,067
1,060
1,044
1,038
1,021
1,014
0,998
0,991
0,931
0,924
0,005
O=S=O
N
2,0
2,0
1,0
5,1
1,1
ppm
9,5
9
8,5
8
7,5
7
6,5
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1
0,5
0
-0,5
-1

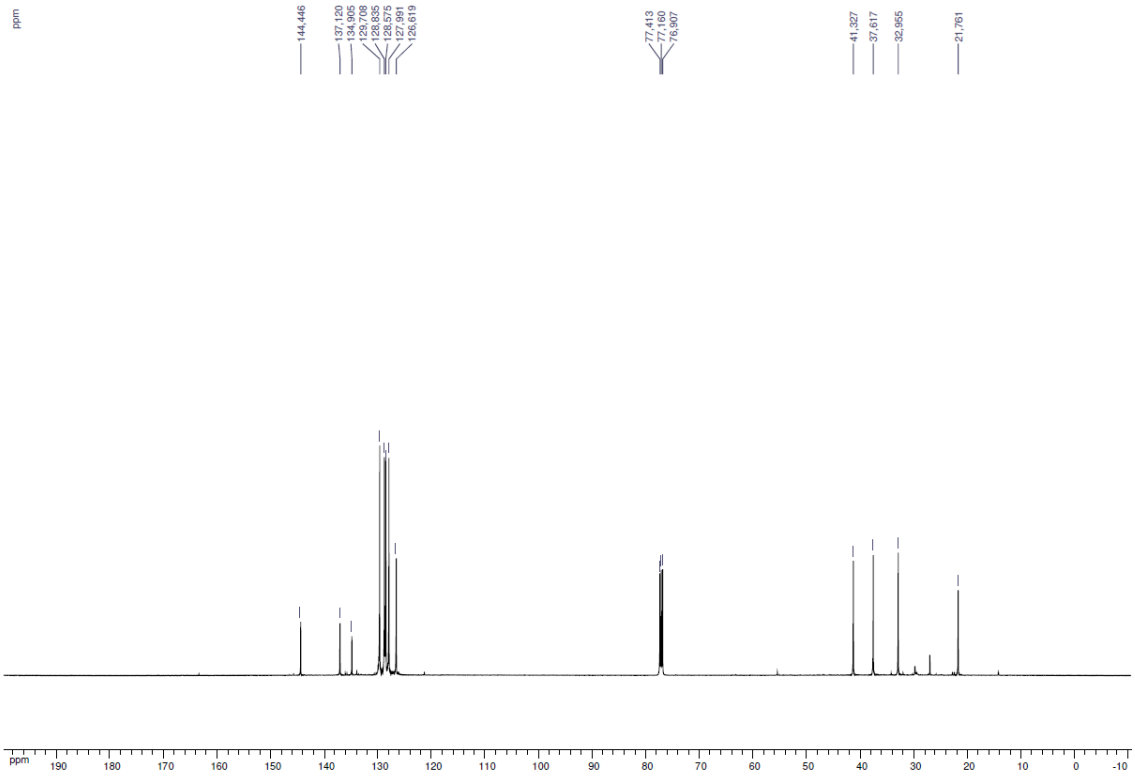
5g

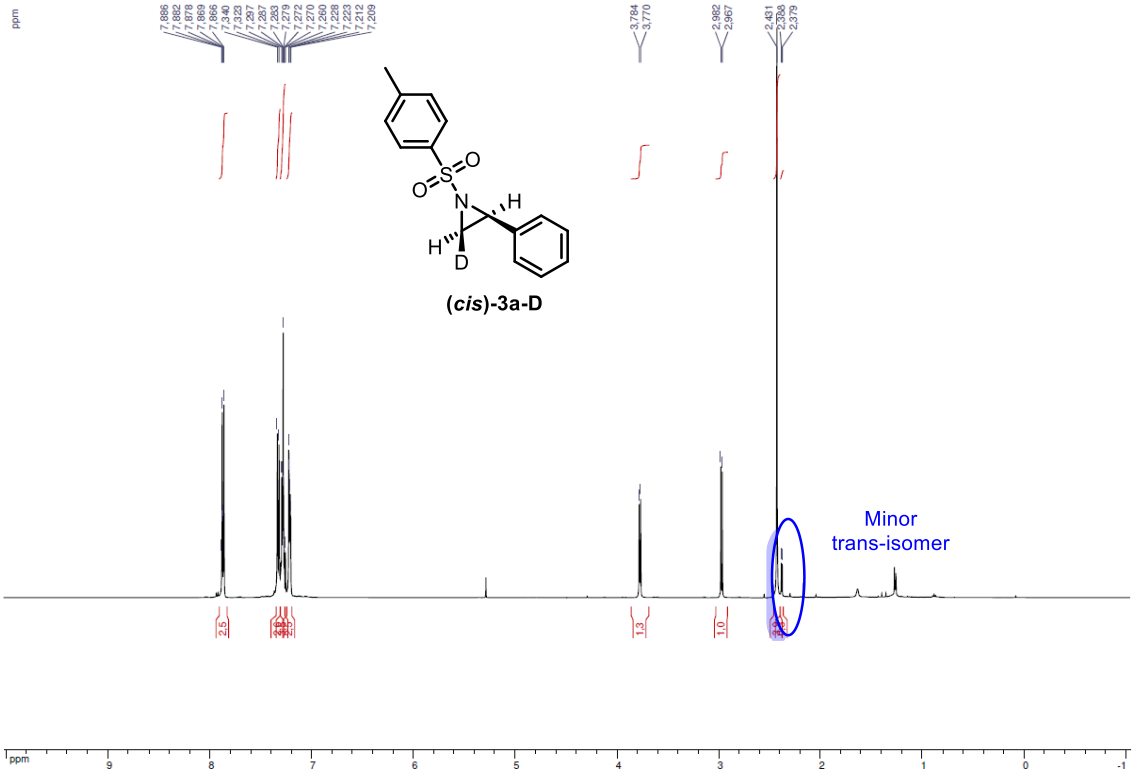

ppm
144,525
135,165
129,708
128,166
77,420
77,160
76,907
45,296
39,508
32,796
30,306
29,736
26,120
25,673
25,485
21,790
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

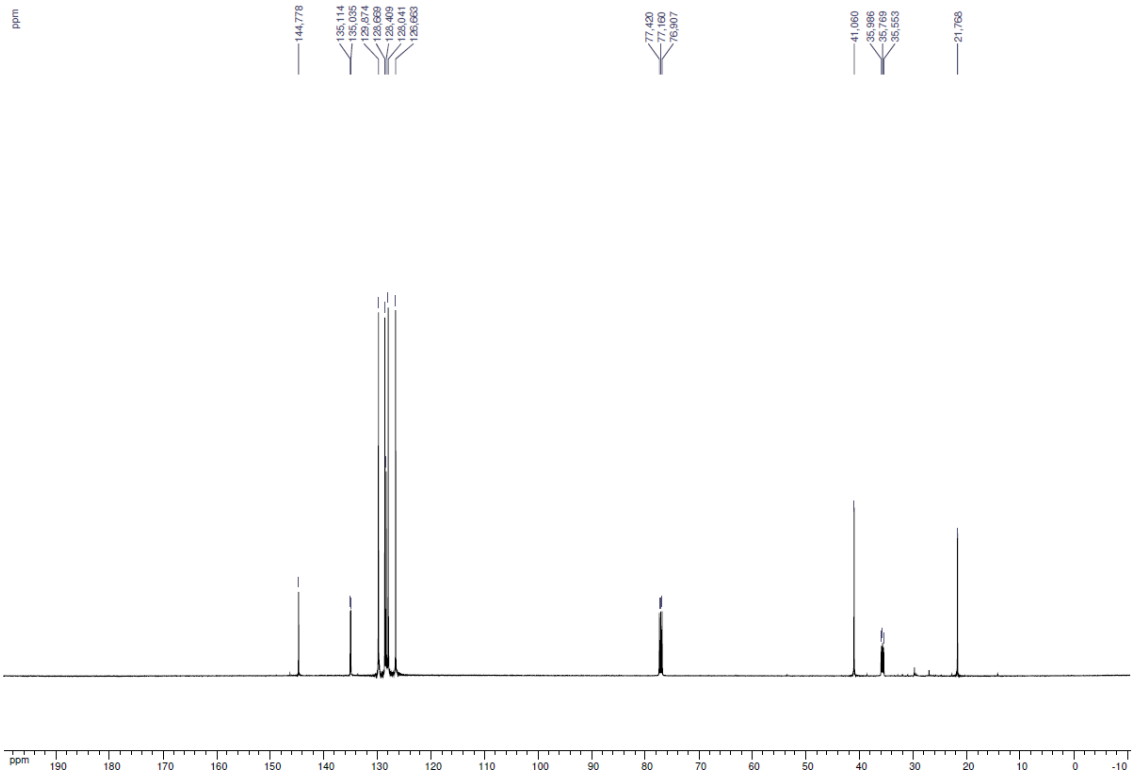

7.697
7.694
7.681
7.260
7.224
7.207
7.165
7.161
7.155
7.151
7.054
7.050
7.043
7.035
2.966
2.961
2.956
2.952
2.948
2.942
2.938
2.928
2.829
2.818
2.800
2.789
2.718
2.714
2.704
2.700
2.685
2.671
2.424
2.418
2.164
2.155
O=S=O
N

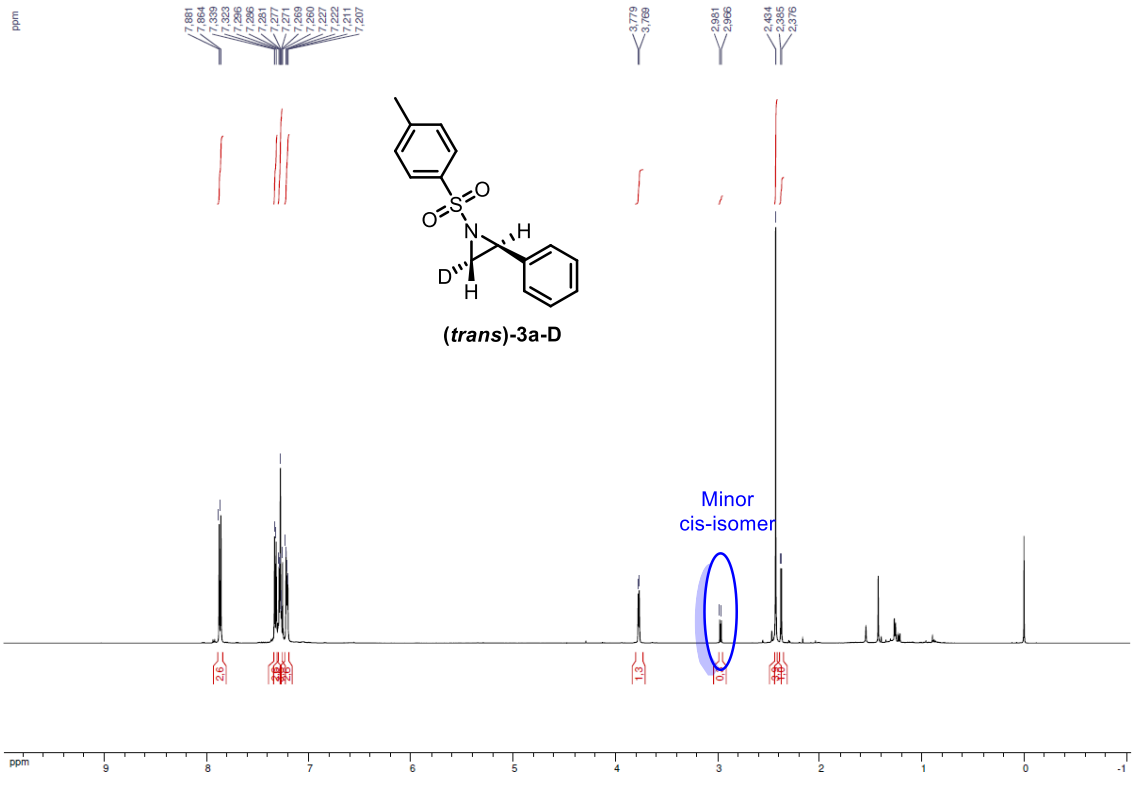
5h


2.0
2.0
2.0
1.0
1.0
2.0
3.0
1.0
ppm
9
8
7
6
5
4
3
2
1
0


144.446
137.120
134.905
129.708
128.835
128.575
127.991
126.619
77.413
77.160
76.907
41.327
37.617
32.955
21.761
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


(cis)-3a-D
Minor
trans-isomer





(*trans*)-3a-D