Supporting Information

Iodine-mediated aminosulfonylation of alkenyl sulfonamides with sulfonyl hydrazides: Synthesis of sulfonylmethyl pyrazolines and pyrrolidines

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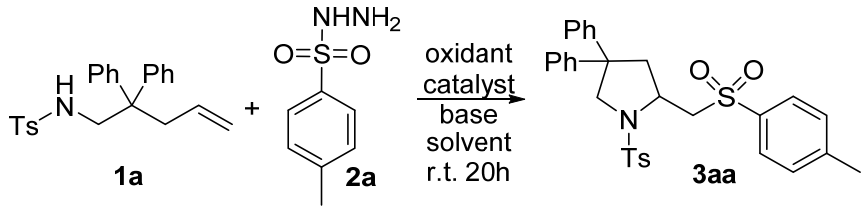
Contents

1. Optimization of Reaction Conditions

Table S1. Optimization of reaction conditions to synthesize sulfone pyrrolidines.[a]

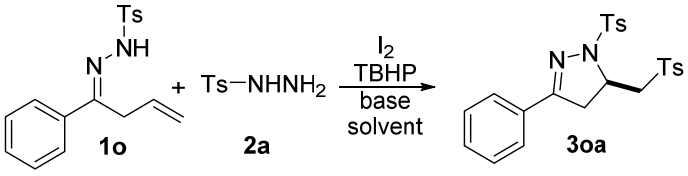


entry	base	solvent	oxidant	catalyst	yield (%)[b]
1	K_2CO_3	1,4-dioxane	TBHP	I_2	20
2	NaOAc	1,4-dioxane	TBHP	I_2	71
3	KF	1,4-dioxane	TBHP	I_2	N.R[c]
4	$NaHCO_3$	1,4-dioxane	TBHP	I_2	79
5	DBU	1,4-dioxane	TBHP	I_2	N.R
6	Na_2CO_3	1,4-dioxane	TBHP	I_2	95
7	*t*-BuOK	1,4-dioxane	TBHP	I_2	N.R
8	Na_2CO_3	1,4-dioxane	TBHP	NaI	82
9	Na_2CO_3	1,4-dioxane	TBHP	NIS	87
10	Na_2CO_3	1,4-dioxane	TBHP	KI	75
11	Na_2CO_3	1,4-dioxane	TBHP	FeI_2	35
12	Na_2CO_3	1,4-dioxane	TBHP	MnI_2	54
13	Na_2CO_3	1,4-dioxane	TBHP	CuI	trace
14	Na_2CO_3	1,4-dioxane	TBHP	TBAI	22
15	None	1,4-dioxane	TBHP	I_2	N.R
16	Na_2CO_3	1,4-dioxane	$K_2S_2O_8$	I_2	trace
17	Na_2CO_3	1,4-dioxane	DTBP	I_2	trace
18	Na_2CO_3	1,4-dioxane	PIDA	I_2	N.R
19	Na_2CO_3	1,4-dioxane	H_2O_2	I_2	N.R
20	Na_2CO_3	THF	TBHP	I_2	81
21	Na_2CO_3	toluene	TBHP	I_2	45
22	Na_2CO_3	MeCN	TBHP	I_2	61
23	Na_2CO_3	acetone	TBHP	I_2	47
24	Na_2CO_3	DCE	TBHP	I_2	63
25	Na_2CO_3	DMF	TBHP	I_2	15
26[d]	NaOAc	1,4-dioxane	TBHP	-	0
27[e]	NaOAc	1,4-dioxane	TBHP	I_2	27

entry	base	solvent	oxidant	catalyst	yield (%)[b]
28[f]	NaOAc	1,4-dioxane	TBHP	I_2	41
29[g]	NaOAc	1,4-dioxane	TBHP	I_2	0

Reaction conditions: [a]**1a** (0.25 mmol), **2a** (0.5 mmol, 2.0 equiv), oxidant (3.0 equiv), solvent (2.0 mL), base (1.5 equiv), catalyst (0.3 equiv), under argon and stirred at room temperature for 20 h. TBHP= *tert*-butyl hydroperoxide (70% aqueous solution), DTBP= Di-*tert*-butyl peroxide , PIDA= (Diacetoxyiodo)benzene. [b]Isolated yield based on **1a**.[c]N.R=No reaction. [d] reaction in the absence of iodine. [e] 10 mol% of iodine was used. [f] 20 mol% of iodine was used. [g] the reaction was carried out in open air system.

Table S2. Optimization of reaction conditions to synthesize sulfone pyrazolines.[a]



entry	base	solvent	oxidant	catalyst	yield (%)[b]
1	Na_2CO_3	1,4-dioxane	TBHP	I_2	23
2	NaOAc	1,4-dioxane	TBHP	I_2	55
3	KF	1,4-dioxane	TBHP	I_2	N.R[c]
4	$NaHCO_3$	1,4-dioxane	TBHP	I_2	75
5	DBU	1,4-dioxane	TBHP	I_2	N.R
6	K_2CO_3	1,4-dioxane	TBHP	I_2	trace
7	CsF	1,4-dioxane	TBHP	I_2	N.R
8	$NaHCO_3$	MeCN	TBHP	I_2	40
9	$NaHCO_3$	DCE	TBHP	I_2	37
10	$NaHCO_3$	Toluene	TBHP	I_2	15
11	$NaHCO_3$	MeCN/H_2O (1:1)	TBHP	I_2	33

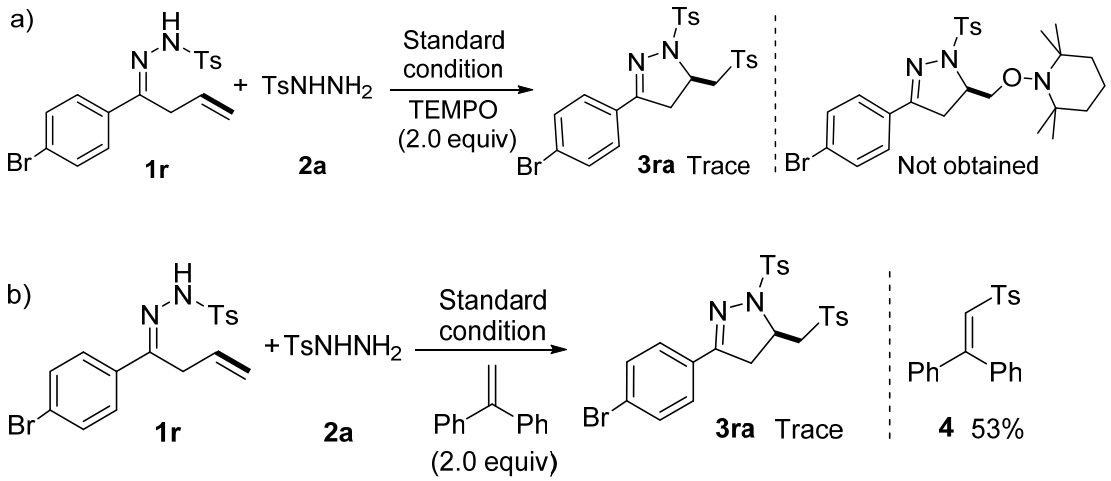
entry	base	solvent	oxidant	catalyst	yield (%)[b]
12	$NaHCO_3$	THF	TBHP	I_2	51
13[d]	$NaHCO_3$	1,4-dioxane	TBHP	I_2	0
14[e]	$NaHCO_3$	1,4-dioxane	TBHP	I_2	22
15[f]	$NaHCO_3$	1,4-dioxane	TBHP	I_2	36

Reaction conditions: [a]**1o** (0.25 mmol), **2a** (0.5 mmol, 2.0 equiv), TBHP (70% aqueous solution, 0.75 mmol, 3.0 equiv), solvent (2.0 mL), base (1.5 equiv), catalyst (0.3 equiv), under argon and stirred at room temperature for 20 h. [b]Isolated yield based on **1o**.[c]N.R=No reaction. [d] reaction carried out in the absence of iodine. [e] 10 mol% of iodine was used. [f] 20 mol% of iodine was used.

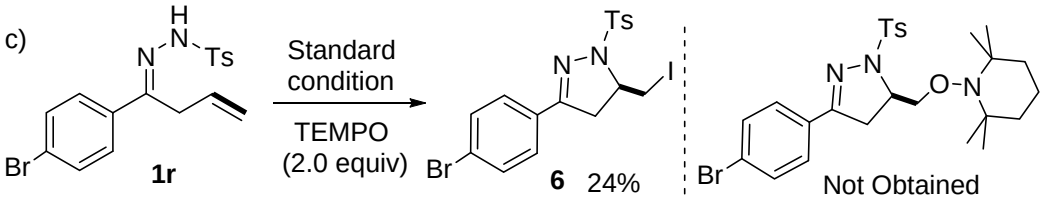
2. Control Reactions Using β,γ-Unsaturated Hydrazone 1r as the Substrate

The control reactions were proceeded using β,γ-unsaturated hydrazone **1r** as substrate and the reaction results did confirm with the results showed in scheme 2, implying that the sulfone pyrazolines and pyrrolidines might be synthesized in the same reaction path way.

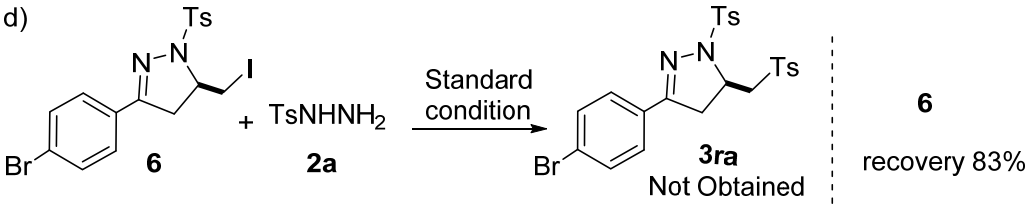
Scheme S1. Control Reactions.



c)

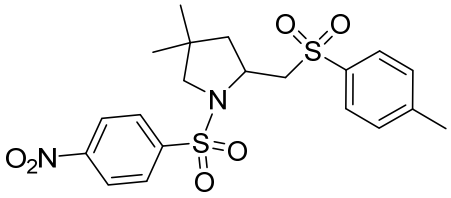

Standard
condition
TEMPO
(2.0 equiv)
1r
6 24%
Not Obtained

d)


6
TsNHNH2
2a
Standard
condition
3ra
Not Obtained
6
recovery 83%

3. X-ray Diffraction Data for 3ga and 3qa

The crystals of **3ga** was obtained by crystallization from a solution in acetone/petroleum ether after purification by column chromatography.



Chemical Formula: $C_{20}H_{24}N_2O_6S_2$

3ga

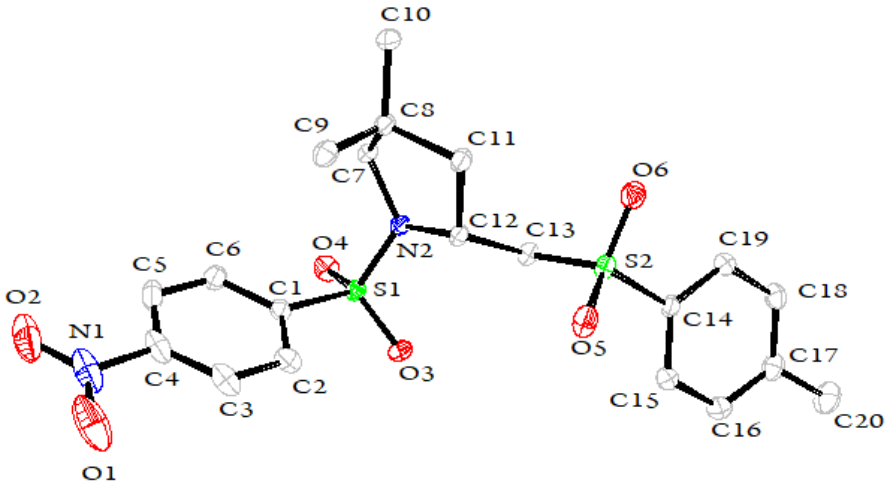


Figure S1. ORTEP drawing of compound **3ga**.

Table S3. Crystal data and structure refinement for **3ga**.

Identification code	3ga
Empirical formula	$C_{20}H_{24}N_2O_6S_2$
Formula weight	452.53
Temperature/K	113
Crystal system	monoclinic
Space group	P 21/c
a/Å	11.026(2)
b/Å	15.703(3)
c/Å	12.684(3)
α/°	90

β/°	98.83(3)
γ/°	90
Volume/Å^3	2170.0(8)
Z	4
ρ_{calc}g/ cm^3	1.385
μ/mm^{-1}	0.284
F (000)	952.0
Crystal size/mm^3	0.200×0.180×0.120
Radiation	MoK\a (0.71073)
2Θ range for data collection/°	2.275 to 27.893
Index ranges	-14 ≤ h ≤ 13, -20≤ k ≤20, -16 ≤ l ≤ 16
Reflections collected	24978
Independent reflections	5168[$R_{(int)}$ = 0.0570]
Data/restraints/parameters	5168/0/275
Goodness-of-fit on F^2	1.084
Final R indexes [I>=2σ (I)]	R1 = 0.0644, wR2 = 0.1619
Final R indexes [all data]	R1 = 0.0775, wR2 = 0.1720
Largest diff. peak/hole / e Å^{-3}	0.445/ -0.401
Flack parameter	n/a

Table S4. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **3ga**. Ueq is defined as 1/3 of the trace of the orthogonalized.

Atom	*x*	*y*	*z*	Ueq
S(1)	4972(1)	2292(1)	1366(1)	26(1)
S(2)	2555(1)	4736(1)	-476(1)	30(1)
O(1)	10878(2)	3281(2)	2502(3)	99(1)
O(2)	10694(3)	2554(2)	3935(3)	89(1)
O(3)	4890(2)	2380(1)	230(1)	35(1)
O(4)	4651(2)	1505(1)	1826(2)	37(1)

Atom	*x*	*y*	*z*	Ueq
O(5)	3693(2)	5010(1)	-780(2)	43(1)
O(6)	1916(2)	5319(1)	132(2)	41(1)
N(1)	10277(3)	2871(2)	3067(3)	67(1)
N(2)	4123(2)	3031(1)	1751(2)	24(1)
C(1)	6532(2)	2475(2)	1907(2)	28(1)
C(2)	7240(2)	2983(2)	1340(2)	37(1)
C(3)	8464(3)	3115(2)	1734(3)	46(1)
C(4)	8950(3)	2739(2)	2676(3)	47(1)
C(5)	8269(3)	2238(2)	3268(3)	48(1)
C(6)	7030(3)	2100(2)	2872(2)	36(1)
C(7)	4024(2)	3134(2)	2901(2)	27(1)
C(8)	4257(2)	4091(2)	3114(2)	28(1)
C(9)	5646(3)	4278(2)	3343(2)	35(1)
C(10)	3630(3)	4417(2)	4031(2)	39(1)
C(11)	3680(3)	4482(2)	2041(2)	32(1)
C(12)	3926(2)	3861(2)	1166(2)	26(1)
C(13)	2844(2)	3761(2)	249(2)	28(1)
C(14)	1554(2)	4464(2)	-1651(2)	28(1)
C(15)	2032(2)	4115(2)	-2503(2)	36(1)
C(16)	1251(3)	3947(2)	-3451(2)	41(1)
C(17)	2(3)	4135(2)	-3557(2)	38(1)
C(18)	-452(2)	4480(2)	-2690(2)	37(1)
C(19)	306(2)	4646(2)	-1729(2)	33(1)
C(20)	-849(3)	3970(2)	-4592(3)	56(1)

Table S5. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3ga.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12

Atom	U11	U22	U33	U23	U13	U12
S(1)	29(1)	25(1)	24(1)	-3(1)	2(1)	-1(1)
S(2)	30(1)	32(1)	26(1)	5(1)	-1(1)	-2(1)
O(1)	34(1)	81(2)	176(4)	9(2)	-1(2)	-9(1)
O(2)	55(2)	88(2)	110(3)	-33(2)	-32(2)	22(2)
O(3)	41(1)	43(1)	22(1)	-7(1)	3(1)	4(1)
O(4)	38(1)	24(1)	49(1)	-1(1)	7(1)	-4(1)
O(5)	30(1)	52(1)	44(1)	18(1)	-2(1)	-12(1)
O(6)	52(1)	37(1)	32(1)	-4(1)	-1(1)	9(1)
N(1)	36(2)	48(2)	110(3)	-14(2)	-10(2)	8(1)
N(2)	27(1)	25(1)	21(1)	0(1)	4(1)	1(1)
C(1)	31(1)	25(1)	28(1)	-2(1)	3(1)	6(1)
C(2)	33(1)	32(1)	47(2)	2(1)	12(1)	2(1)
C(3)	31(1)	32(2)	75(2)	-2(2)	10(1)	1(1)
C(4)	29(1)	38(2)	72(2)	-13(2)	-2(1)	6(1)
C(5)	45(2)	48(2)	43(2)	-8(1)	-12(1)	18(1)
C(6)	39(1)	37(1)	32(1)	1(1)	2(1)	4(1)
C(7)	31(1)	31(1)	19(1)	1(1)	3(1)	2(1)
C(8)	36(1)	27(1)	22(1)	-2(1)	1(1)	6(1)
C(9)	42(1)	32(1)	30(1)	-4(1)	0(1)	-3(1)
C(10)	49(2)	41(2)	27(1)	-4(1)	6(1)	15(1)
C(11)	41(1)	28(1)	25(1)	-1(1)	-1(1)	6(1)
C(12)	27(1)	28(1)	22(1)	3(1)	2(1)	-1(1)
C(13)	30(1)	29(1)	25(1)	2(1)	0(1)	-2(1)
C(14)	25(1)	32(1)	24(1)	6(1)	1(1)	1(1)
C(15)	29(1)	45(2)	34(1)	1(1)	4(1)	7(1)
C(16)	44(2)	48(2)	31(1)	-5(1)	6(1)	6(1)
C(17)	41(2)	36(1)	33(1)	1(1)	-4(1)	-3(1)
C(18)	27(1)	42(2)	39(2)	1(1)	-4(1)	3(1)

Atom	U11	U22	U33	U23	U13	U12
C(19)	28(1)	38(1)	33(1)	2(1)	5(1)	4(1)
C(20)	56(2)	63(2)	41(2)	-5(2)	-14(2)	-4(2)

Table S6. Bond lengths for **3ga.**

Atom	Length/Å	Atom	Length/Å
S(1)-O(4)	1.4332(19)	C(3)-C(4)	1.366(5)
S(1)-O(3)	1.4355(19)	C(4)-C(5)	1.386(5)
S(1)-N(2)	1.613(2)	C(5)-C(6)	1.398(4)
S(1)-C(1)	1.775(3)	C(7)-C(8)	1.541(3)
S(2)-O(5)	1.4343(19)	C(8)-C(10)	1.531(3)
S(2)-O(6)	1.448(2)	C(8)-C(11)	1.539(3)
S(2)-C(14)	1.765(3)	C(8)-C(9)	1.542(4)
S(2)-C(13)	1.788(3)	C(11)-C(12)	1.533(3)
O(1)-N(1)	1.230(5)	C(12)-C(13)	1.540(3)
O(2)-N(1)	1.231(5)	C(14)-C(15)	1.386(4)
N(1)-C(4)	1.486(4)	C(14)-C(19)	1.394(3)
N(2)-C(7)	1.488(3)	C(15)-C(16)	1.393(4)
N(2)-C(12)	1.500(3)	C(16)-C(17)	1.394(4)
C(1)-C(2)	1.391(4)	C(17)-C(18)	1.386(4)
C(1)-C(6)	1.392(4)	C(17)-C(20)	1.515(4)
C(2)-C(3)	1.381(4)	C(18)-C(19)	1.393(4)

Table S7. Bond angles for **3ga.**

Atom	Angle/°	Atom	Angle/°
O(4)-S(1)-O(3)	120.70(12)	C(5)-C(4)-N(1)	119.1(3)
O(4)-S(1)-N(2)	107.77(11)	C(4)-C(5)-C(6)	118.3(3)
O(3)-S(1)-N(2)	106.54(11)	C(1)-C(6)-C(5)	118.9(3)

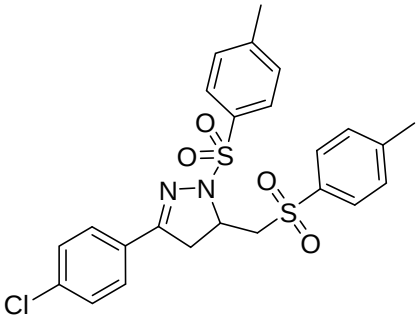
Atom	Angle/°	Atom	Angle/°
O(4)-S(1)-C(1)	105.48(12)	N(2)-C(7)-C(8)	104.06(19)
O(3)-S(1)-C(1)	106.26(12)	C(10)-C(8)-C(11)	111.4(2)
N(2)-S(1)-C(1)	109.85(11)	C(10)-C(8)-C(7)	112.1(2)
O(5)-S(2)-O(6)	118.04(13)	C(11)-C(8)-C(7)	101.49(19)
O(5)-S(2)-C(14)	107.82(12)	C(10)-C(8)-C(9)	110.1(2)
O(6)-S(2)-C(14)	108.05(12)	C(11)-C(8)-C(9)	110.8(2)
O(5)-S(2)-C(13)	107.54(12)	C(7)-C(8)-C(9)	110.7(2)
O(6)-S(2)-C(13)	109.24(12)	C(12)-C(11)-C(8)	106.9(2)
C(14)-S(2)-C(13)	105.45(12)	N(2)-C(12)-C(11)	102.87(18)
O(1)-N(1)-O(2)	124.9(3)	N(2)-C(12)-C(13)	108.78(19)
O(1)-N(1)-C(4)	118.0(4)	C(11)-C(12)-C(13)	114.1(2)
O(2)-N(1)-C(4)	117.1(4)	C(12)-C(13)-S(2)	110.94(17)
C(7)-N(2)-C(12)	111.27(18)	C(15)-C(14)-C(19)	121.0(2)
C(7)-N(2)-S(1)	120.63(16)	C(15)-C(14)-S(2)	119.33(19)
C(12)-N(2)-S(1)	121.47(16)	C(19)-C(14)-S(2)	119.5(2)
C(2)-C(1)-C(6)	121.3(2)	C(14)-C(15)-C(16)	119.3(2)
C(2)-C(1)-S(1)	118.7(2)	C(15)-C(16)-C(17)	120.9(3)
C(6)-C(1)-S(1)	120.0(2)	C(18)-C(17)-C(16)	118.6(3)
C(3)-C(2)-C(1)	119.6(3)	C(18)-C(17)-C(20)	120.2(3)
C(4)-C(3)-C(2)	118.8(3)	C(16)-C(17)-C(20)	121.2(3)
C(3)-C(4)-C(5)	123.2(3)	C(17)-C(18)-C(19)	121.7(2)
C(3)-C(4)-N(1)	117.8(3)	C(18)-C(19)-C(14)	118.5(3)

Table S8. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3ga.**

Atom	*x*	*y*	*z*	Ueq
H(2)	6883	3238	687	44
H(3)	8960	3461	1357	55

Atom	*x*	*y*	*z*	Ueq
H(5)	8634	1994	3926	57
H(6)	6536	1757	3254	43
H(7A)	4646	2784	3353	33
H(7B)	3197	2969	3043	33
H(9A)	5776	4892	3435	53
H(9B)	6035	4078	2743	53
H(9C)	6008	3982	3996	53
H(10A)	3702	5039	4075	58
H(10B)	4025	4165	4704	58
H(10C)	2760	4258	3904	58
H(11A)	2786	4561	2022	38
H(11B)	4054	5043	1939	38
H(12)	4686	4031	878	31
H(13A)	2100	3591	544	34
H(13B)	3034	3306	-241	34
H(15)	2883	3991	-2440	43
H(16)	1573	3701	-4034	49
H(18)	-1303	4607	-2754	45
H(19)	-20	4878	-1140	39
H(20A)	-1086	3368	-4631	83
H(20B)	-426	4110	-5196	83
H(20C)	-1584	4324	-4621	83

The crystals of **3qa** was obtained by crystallization from a solution in acetone/petroleum ether after purification by column chromatography.



Chemical Formula: $C_{24}H_{23}ClN_2O_4S_2$

3qa

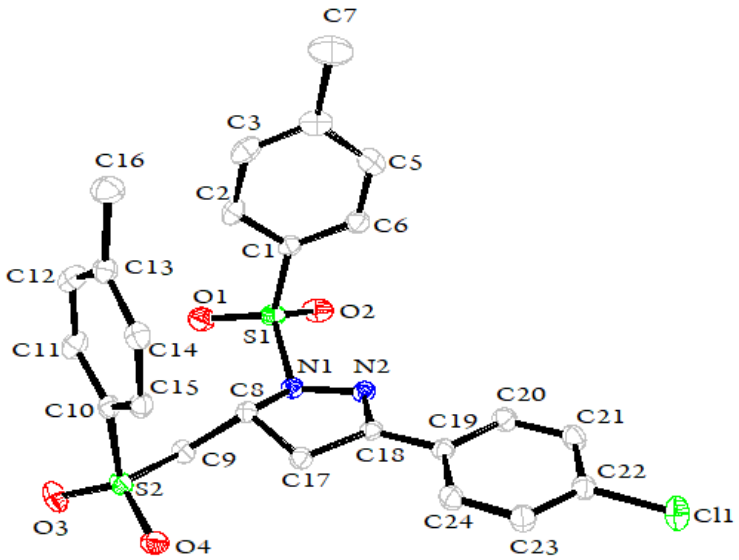


Figure S2. ORTEP drawing of compound **3qa**.

Table S9. Crystal data and structure refinement for **3qa**.

Identification code	3qa
Empirical formula	$C_{24}H_{23}ClN_2O_4S_2$
Formula weight	503.01
Temperature/K	113
Crystal system	Triclinic
Space group	P-1
a/Å	10.622(2)
b/Å	10.722(2)

c/Å	11.698(2)
α/°	78.63(3)
β/°	98.83(3)
γ/°	67.46(3)
Volume/Å^3	1196.0(5)
Z	2
ρ_{calc}g/ cm^3	1.397
μ/mm^{-1}	0.368
F (000)	524
Crystal size/mm^3	0.200×0.180×0.120
Radiation	MoK\a (0.71073)
2Θ range for data collection/°	2.076 to 27.853
Index ranges	-13 ≤ h ≤ 13, -14≤ k ≤14, -15 ≤ l ≤ 15
Reflections collected	14274
Independent reflections	5654 [$R_{(int)}$ = 0.0405]
Data/restraints/parameters	5654 / 0 / 300
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R1 = 0.0424, wR2 = 0.1104
Final R indexes [all data]	R1 = 0.0570, wR2 = 0.1190
Largest diff. peak/hole / e Å^{-3}	0.269/ -0.361
Flack parameter	n/a

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **3qa**. Ueq is defined as 1/3 of the trace of the orthogonalized.

Atom	*x*	*y*	*z*	Ueq
S(1)	9159(1)	-491(1)	2383(1)	33(1)
S(2)	12000(1)	2480(1)	1232(1)	32(1)
Cl(1)	3474(1)	5778(1)	-2764(1)	46(1)

Atom	*x*	*y*	*z*	Ueq
O(1)	10424(1)	-880(1)	2861(1)	44(1)
O(2)	8786(2)	-1495(1)	2035(1)	45(1)
O(3)	13407(1)	1779(1)	1451(1)	46(1)
O(4)	11698(1)	3536(1)	239(1)	38(1)
N(1)	9294(2)	600(1)	1187(1)	29(1)
N(2)	8085(2)	1147(1)	634(1)	30(1)
C(1)	7811(2)	392(2)	3385(1)	30(1)
C(2)	8108(2)	802(2)	4333(2)	36(1)
C(3)	7043(2)	1436(2)	5153(2)	43(1)
C(4)	5690(2)	1671(2)	5049(2)	45(1)
C(5)	5415(2)	1301(2)	4078(2)	43(1)
C(6)	6456(2)	666(2)	3250(2)	36(1)
C(7)	4536(3)	2332(3)	5971(2)	72(1)
C(8)	9776(2)	1724(2)	1276(2)	28(1)
C(9)	11344(2)	1223(2)	1109(2)	32(1)
C(10)	11006(2)	3177(2)	2502(2)	29(1)
C(11)	11161(2)	2373(2)	3590(2)	38(1)
C(12)	10265(2)	2839(2)	4564(2)	42(1)
C(13)	9212(2)	4109(2)	4484(2)	37(1)
C(14)	9115(2)	4920(2)	3402(2)	35(1)
C(15)	9982(2)	4458(2)	2401(2)	32(1)
C(16)	8185(2)	4546(2)	5547(2)	52(1)
C(17)	9077(2)	2826(2)	308(2)	30(1)
C(18)	7958(2)	2367(2)	139(1)	28(1)
C(19)	6852(2)	3189(2)	-572(1)	28(1)
C(20)	5817(2)	2725(2)	-665(2)	36(1)
C(21)	4779(2)	3525(2)	-1334(2)	38(1)
C(22)	4774(2)	4786(2)	-1910(2)	33(1)

Atom	*x*	*y*	*z*	Ueq
C(23)	5767(2)	5273(2)	-1813(2)	37(1)
C(24)	6803(2)	4462(2)	-1138(2)	36(1)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3qa.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U11	U22	U33	U23	U13	U12
S(1)	38(1)	26(1)	31(1)	-1(1)	0(1)	-11(1)
S(2)	30(1)	35(1)	35(1)	-7(1)	-1(1)	-14(1)
Cl(1)	36(1)	43(1)	58(1)	-6(1)	-18(1)	-8(1)
O(1)	36(1)	42(1)	42(1)	8(1)	-5(1)	-7(1)
O(2)	63(1)	30(1)	43(1)	-7(1)	6(1)	-24(1)
O(3)	26(1)	51(1)	62(1)	-13(1)	-4(1)	-13(1)
O(4)	45(1)	40(1)	33(1)	-3(1)	1(1)	-23(1)
N(1)	35(1)	28(1)	27(1)	-3(1)	-3(1)	-15(1)
N(2)	35(1)	31(1)	25(1)	-5(1)	-3(1)	-15(1)
C(1)	36(1)	26(1)	26(1)	1(1)	-4(1)	-13(1)
C(2)	44(1)	31(1)	33(1)	1(1)	-14(1)	-11(1)
C(3)	64(1)	31(1)	32(1)	-6(1)	-10(1)	-10(1)
C(4)	53(1)	31(1)	42(1)	-5(1)	6(1)	-10(1)
C(5)	36(1)	39(1)	50(1)	-4(1)	0(1)	-14(1)
C(6)	41(1)	39(1)	32(1)	-2(1)	-5(1)	-21(1)
C(7)	76(2)	54(2)	67(2)	-26(1)	24(1)	-10(1)
C(8)	32(1)	28(1)	26(1)	-7(1)	-2(1)	-12(1)
C(9)	32(1)	30(1)	35(1)	-9(1)	-1(1)	-11(1)
C(10)	31(1)	30(1)	31(1)	-6(1)	-6(1)	-14(1)
C(11)	49(1)	30(1)	36(1)	-1(1)	-14(1)	-12(1)
C(12)	62(1)	38(1)	30(1)	-2(1)	-9(1)	-23(1)
C(13)	44(1)	47(1)	32(1)	-12(1)	-2(1)	-25(1)

Atom	U11	U22	U33	U23	U13	U12
C(14)	32(1)	34(1)	40(1)	-9(1)	-5(1)	-11(1)
C(15)	34(1)	32(1)	32(1)	0(1)	-9(1)	-15(1)
C(16)	60(1)	64(2)	41(1)	-20(1)	6(1)	-32(1)
C(17)	34(1)	31(1)	29(1)	-2(1)	-4(1)	-15(1)
C(18)	34(1)	31(1)	21(1)	-7(1)	0(1)	-16(1)
C(19)	32(1)	31(1)	23(1)	-8(1)	0(1)	-12(1)
C(20)	41(1)	36(1)	36(1)	-3(1)	-5(1)	-21(1)
C(21)	35(1)	45(1)	43(1)	-8(1)	-4(1)	-23(1)
C(22)	29(1)	36(1)	32(1)	-10(1)	-3(1)	-8(1)
C(23)	39(1)	32(1)	42(1)	1(1)	-9(1)	-15(1)
C(24)	37(1)	36(1)	39(1)	-1(1)	-8(1)	-21(1)

Table S12. Bond lengths for **3qa.**

Atom	Length/Å	Atom	Length/Å
S(1)-O(2)	1.4301(13)	C(5)-C(6)	1.376(3)
S(1)-O(1)	1.4360(14)	C(8)-C(9)	1.527(2)
S(1)-N(1)	1.6582(15)	C(8)-C(17)	1.534(2)
S(1)-C(1)	1.7518(19)	C(10)-C(15)	1.387(2)
S(2)-O(3)	1.4401(14)	C(10)-C(11)	1.389(2)
S(2)-O(4)	1.4429(14)	C(11)-C(12)	1.375(3)
S(2)-C(10)	1.7628(19)	C(12)-C(13)	1.391(3)
S(2)-C(9)	1.7763(18)	C(13)-C(14)	1.384(3)
Cl(1)-C(22)	1.7393(19)	C(13)-C(16)	1.507(3)
N(1)-N(2)	1.4157(19)	C(14)-C(15)	1.388(2)
N(1)-C(8)	1.505(2)	C(17)-C(18)	1.507(2)
N(2)-C(18)	1.288(2)	C(18)-C(19)	1.465(2)
C(1)-C(6)	1.388(2)	C(19)-C(24)	1.381(2)
C(1)-C(2)	1.399(2)	C(19)-C(20)	1.398(2)

Atom	Length/Å	Atom	Length/Å
C(2)-C(3)	1.382(3)	C(20)-C(21)	1.382(3)
C(3)-C(4)	1.386(3)	C(21)-C(22)	1.385(3)
C(4)-C(5)	1.389(3)	C(22)-C(23)	1.375(2)
C(4)-C(7)	1.514(3)	C(23)-C(24)	1.387(3)

Table S13. Bond angles for **3qa.**

Atom	Angle/°	Atom	Angle/°
O(2)-S(1)-O(1)	120.30(9)	C(5)-C(6)-C(1)	119.41(17)
O(2)-S(1)-N(1)	106.79(8)	N(1)-C(8)-C(9)	110.57(13)
O(1)-S(1)-N(1)	104.66(8)	N(1)-C(8)-C(17)	101.09(12)
O(2)-S(1)-C(1)	108.24(9)	C(9)-C(8)-C(17)	115.40(15)
O(1)-S(1)-C(1)	108.27(9)	C(8)-C(9)-S(2)	113.47(12)
N(1)-S(1)-C(1)	108.00(8)	C(15)-C(10)-C(11)	120.39(17)
O(3)-S(2)-O(4)	119.07(9)	C(15)-C(10)-S(2)	120.14(14)
O(3)-S(2)-C(10)	109.14(9)	C(11)-C(10)-S(2)	119.13(14)
O(4)-S(2)-C(10)	107.97(8)	C(12)-C(11)-C(10)	119.54(17)
O(3)-S(2)-C(9)	107.26(9)	C(11)-C(12)-C(13)	121.29(18)
O(4)-S(2)-C(9)	108.89(8)	C(14)-C(13)-C(12)	118.23(17)
C(10)-S(2)-C(9)	103.39(8)	C(14)-C(13)-C(16)	121.75(19)
N(2)-N(1)-C(8)	109.94(12)	C(12)-C(13)-C(16)	119.98(19)
N(2)-N(1)-S(1)	112.06(11)	C(13)-C(14)-C(15)	121.48(17)
C(8)-N(1)-S(1)	118.47(10)	C(10)-C(15)-C(14)	118.94(17)
C(18)-N(2)-N(1)	108.16(14)	C(18)-C(17)-C(8)	101.94(14)
C(6)-C(1)-C(2)	120.12(17)	N(2)-C(18)-C(19)	121.91(15)
C(6)-C(1)-S(1)	120.27(13)	N(2)-C(18)-C(17)	114.16(15)
C(2)-C(1)-S(1)	119.61(14)	C(19)-C(18)-C(17)	123.86(15)
C(3)-C(2)-C(1)	119.26(18)	C(24)-C(19)-C(20)	119.05(17)
C(3)-C(2)-H(2)	120.4	C(24)-C(19)-C(18)	119.73(16)

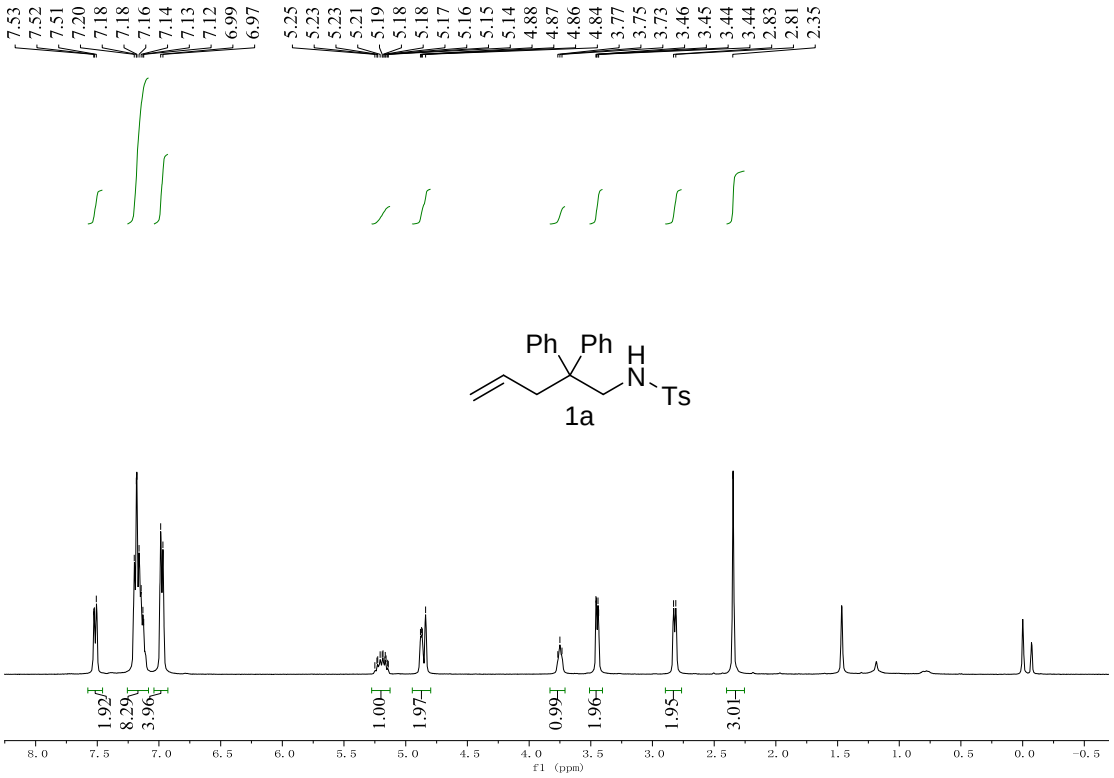
Atom	Angle/°	Atom	Angle/°
C(1)-C(2)-H(2)	120.4	C(20)-C(19)-C(18)	121.20(16)
C(2)-C(3)-C(4)	121.06(18)	C(21)-C(20)-C(19)	120.07(18)
C(2)-C(3)-H(3)	119.5	C(20)-C(21)-C(22)	119.46(17)
C(4)-C(3)-H(3)	119.5	C(23)-C(22)-C(21)	121.46(17)
C(3)-C(4)-C(5)	118.70(18)	C(23)-C(22)-Cl(1)	119.36(15)
C(3)-C(4)-C(7)	120.6(2)	C(21)-C(22)-Cl(1)	119.18(14)
C(5)-C(4)-C(7)	120.7(2)	C(22)-C(23)-C(24)	118.56(18)
C(6)-C(5)-C(4)	121.37(19)	C(19)-C(24)-C(23)	121.38(17)

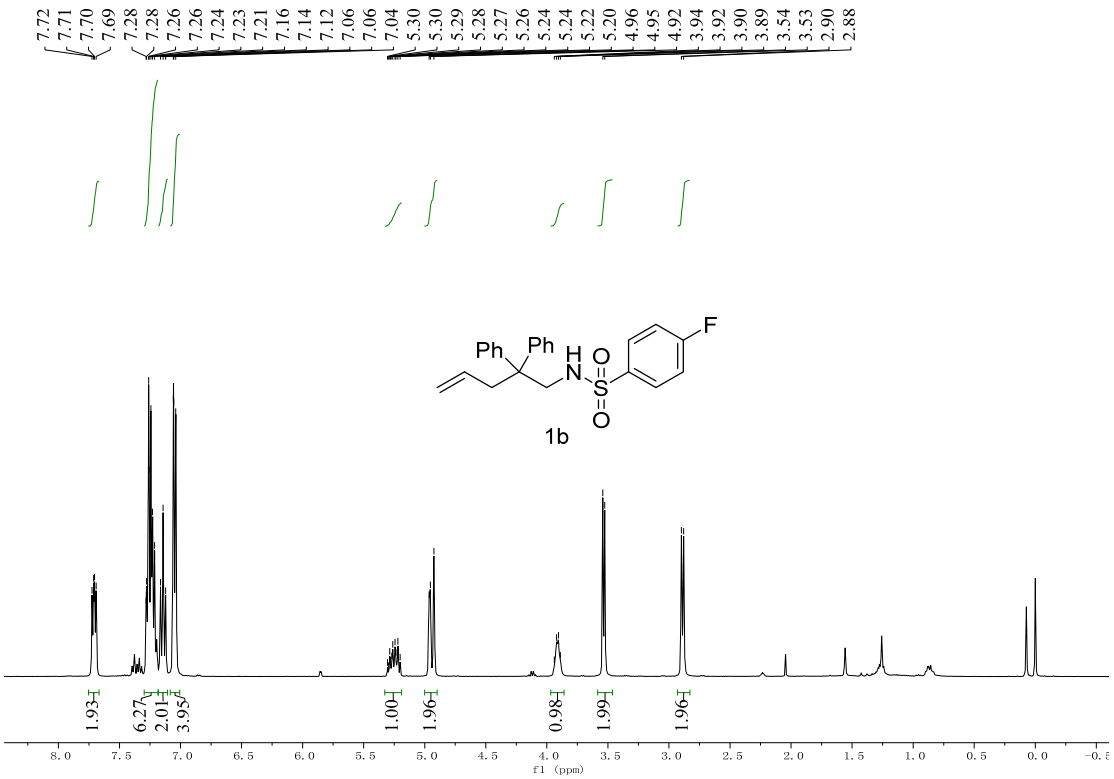
Table S14. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3qa.**

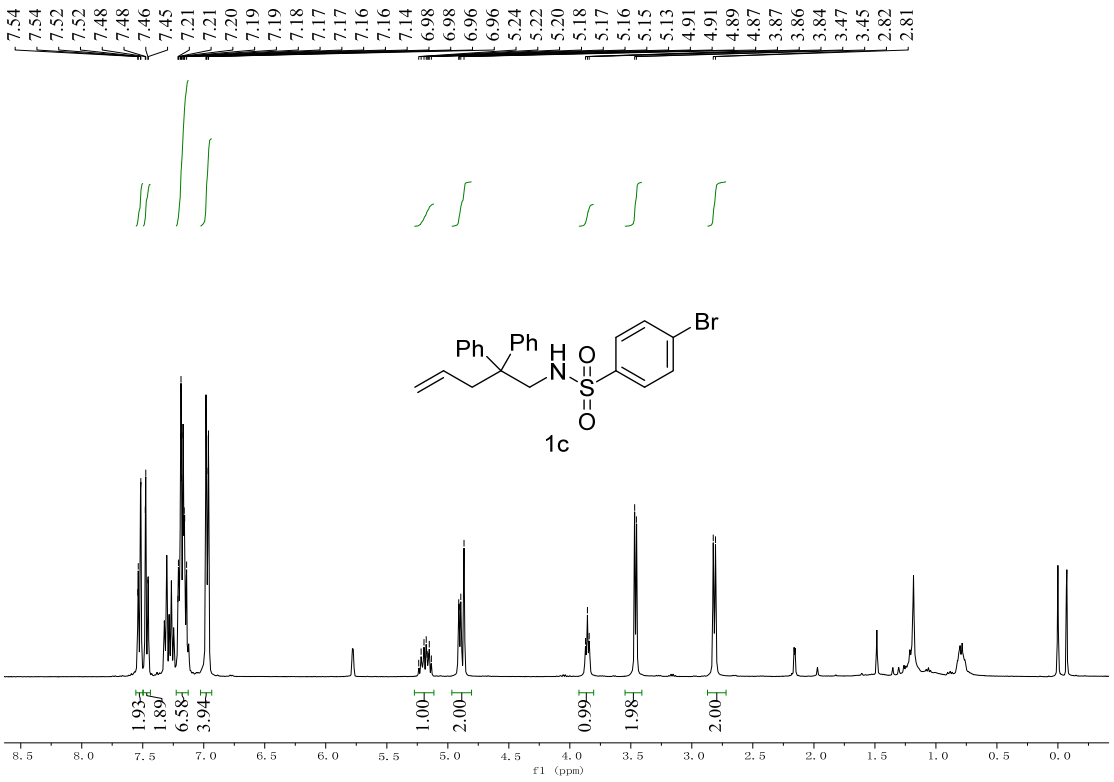
Atom	*x*	*y*	*z*	Ueq
H(2)	9031	647	4412	44
H(3)	7241	1715	5799	52
H(5)	4488	1490	3983	52
H(6)	6250	418	2592	43
H(7A)	4428	3290	5924	108
H(7B)	4753	1855	6754	108
H(7C)	3678	2279	5832	108
H(8)	9405	2051	2060	34
H(9A)	11695	922	323	38
H(9B)	11694	423	1705	38
H(11)	11881	1508	3662	46
H(12)	10368	2283	5305	50
H(14)	8440	5813	3343	42
H(15)	9876	5010	1658	38
H(16A)	7310	4487	5461	78
H(16B)	8042	5488	5617	78

Atom	*x*	*y*	*z*	Ueq
H(16C)	8534	3947	6254	78
H(17A)	8691	3739	566	36
H(17B)	9725	2843	-423	36
H(20)	5828	1859	-268	43
H(21)	4073	3214	-1398	46
H(23)	5743	6147	-2200	45
H(24)	7494	4788	-1064	43

4. Copies of ^{1}H and ^{13}C NMR Spectra.



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Ph
Ph
H
N
O
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O
Br
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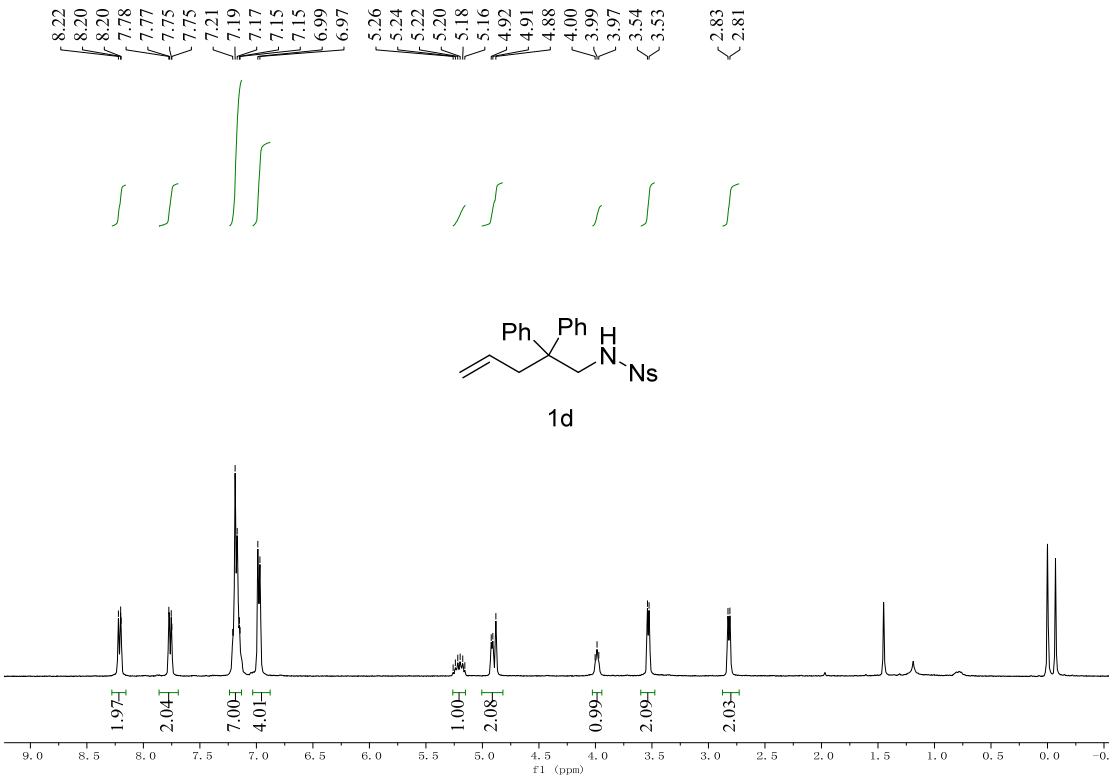
f1 (ppm)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Ph
Ph
H
N
Ns
1d
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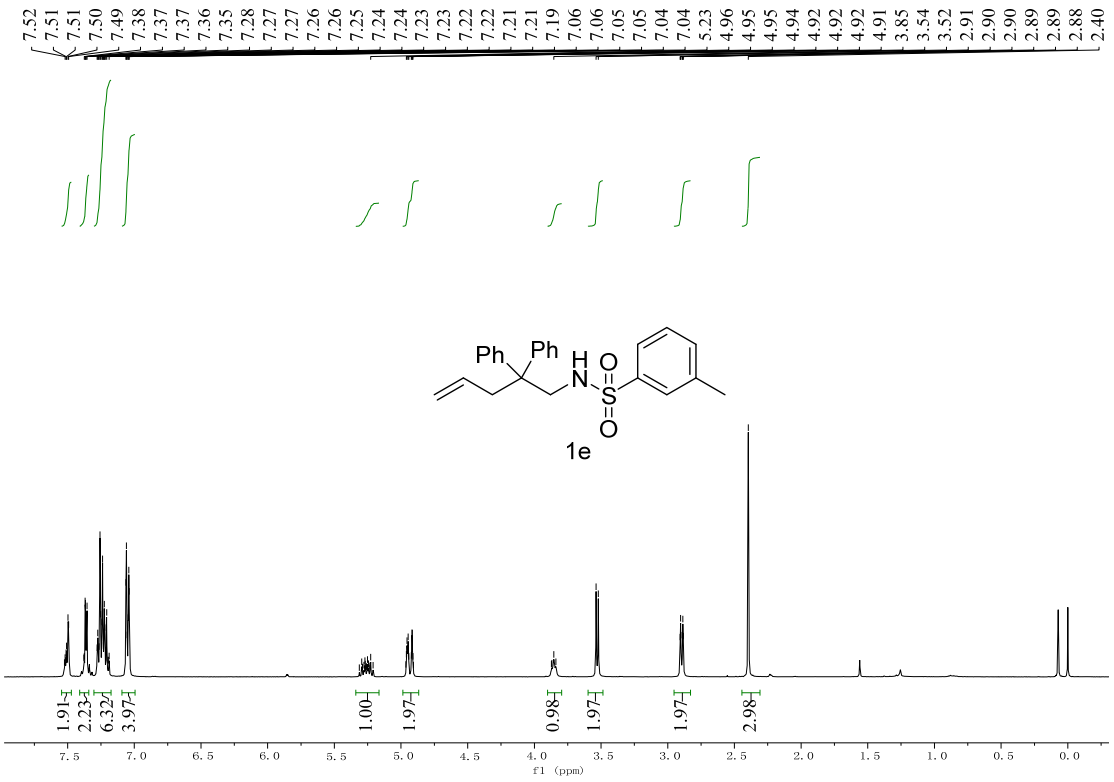
f1 (ppm)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Ph Ph H N O S O O
1e
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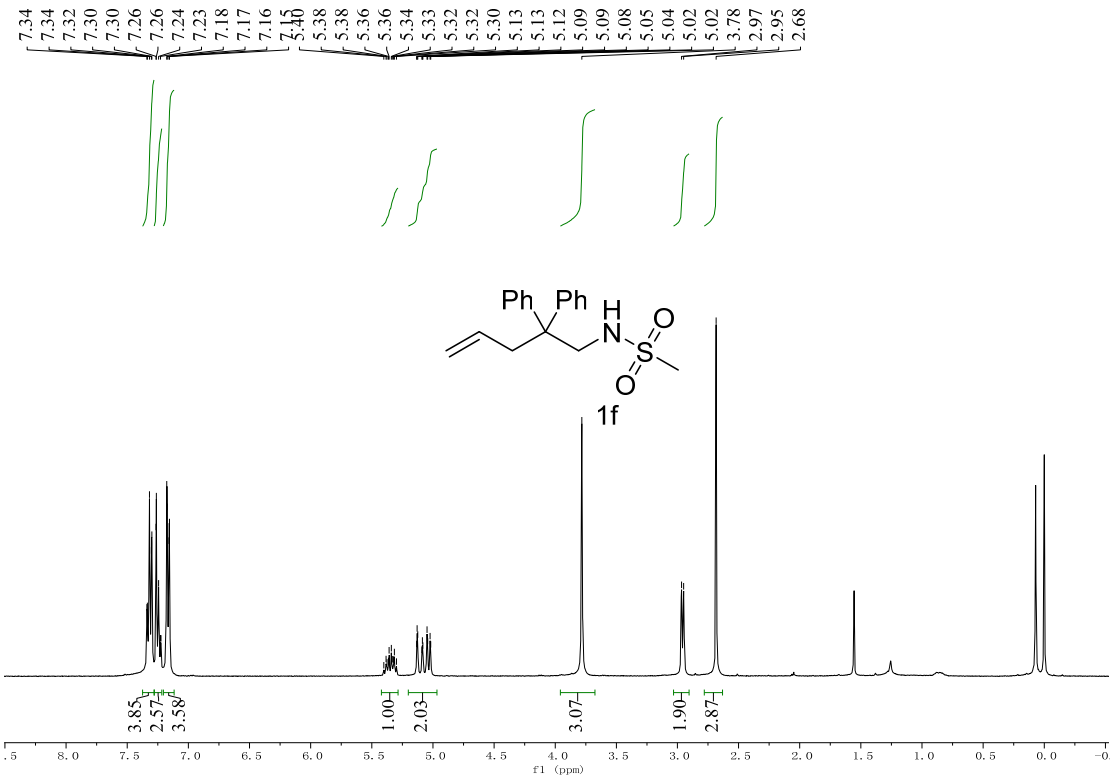
f1 (ppm)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Ph Ph H N O S O O
1f
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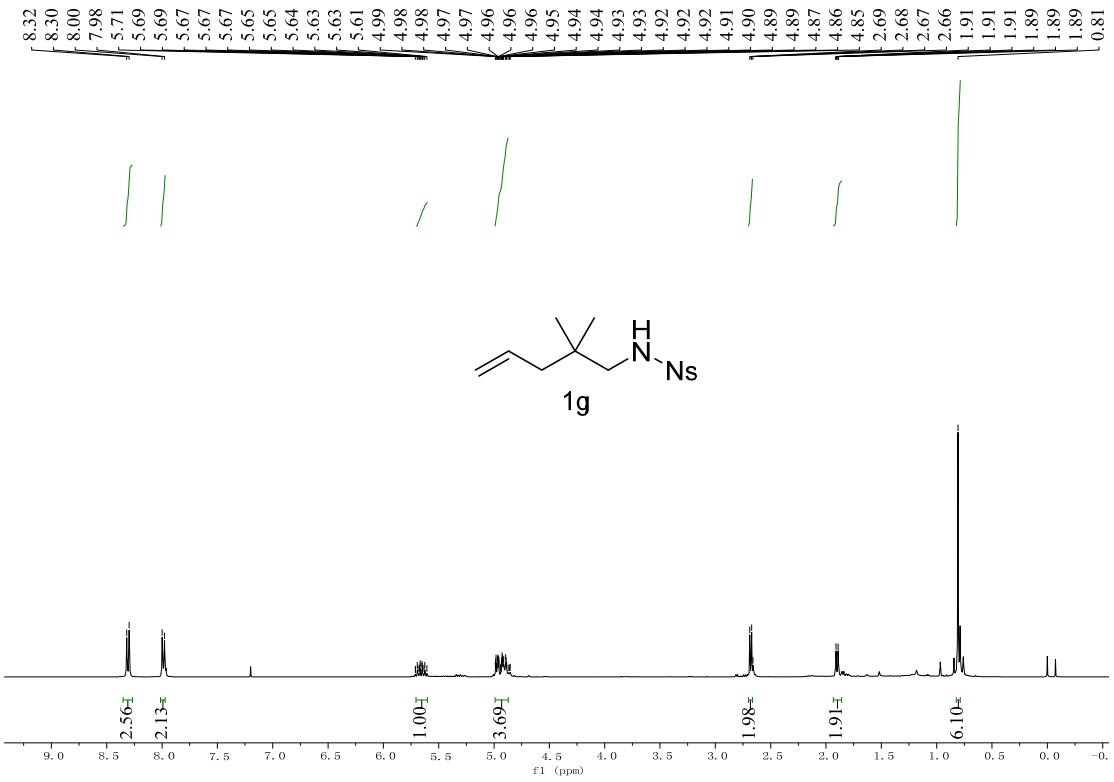
f1 (ppm)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H
N
Ns
1g
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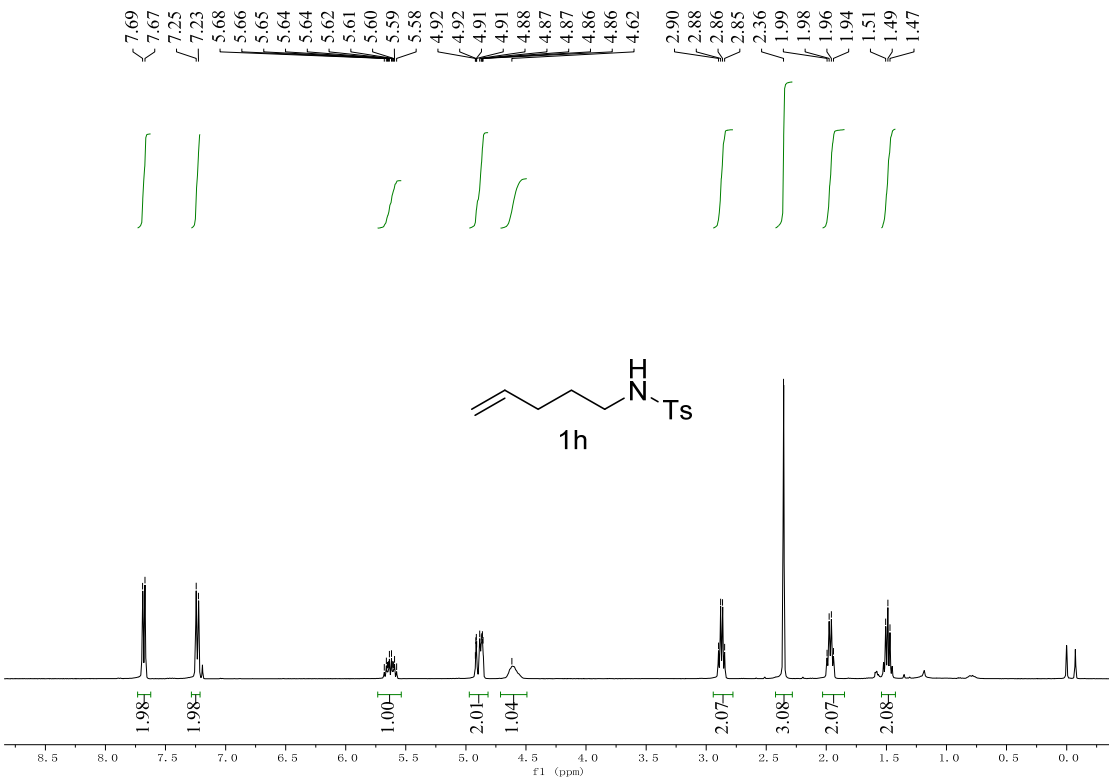
f1 (ppm)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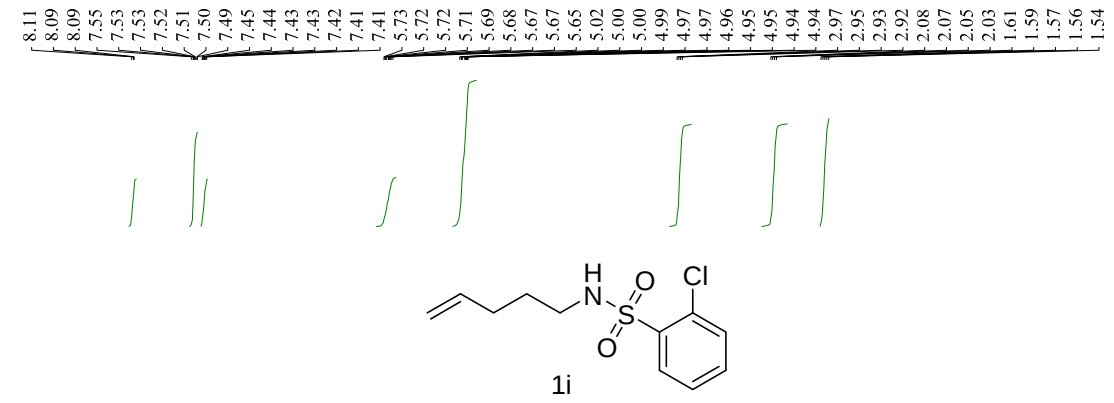
H
N
Ts
1h
1.98 1.98 1.00 2.01 1.04 2.07 3.08 2.07 2.08
f1 (ppm)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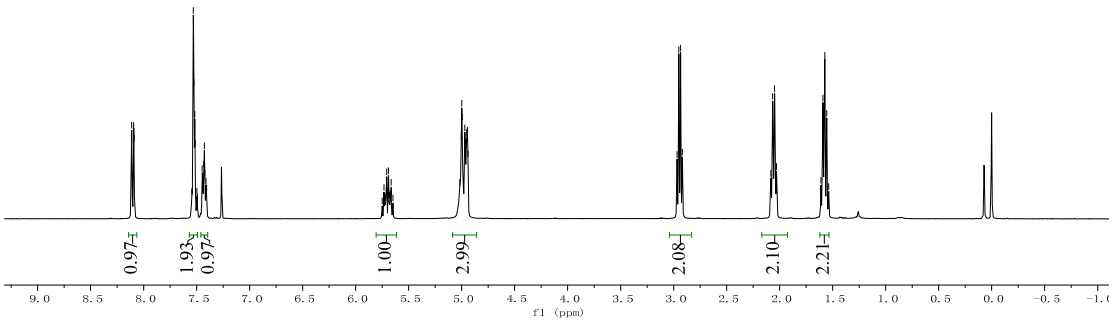
5.73 5.72 5.72 5.71 5.69 5.68 5.67 5.67 5.65 5.02 5.00 5.00 4.99 4.97 4.97 4.96 4.95 4.95 4.94 4.94 2.97 2.95 2.93 2.92 2.08 2.07 2.05 2.03 1.61 1.59 1.57 1.56 1.54
H
N
S
O
O
O
Cl

1i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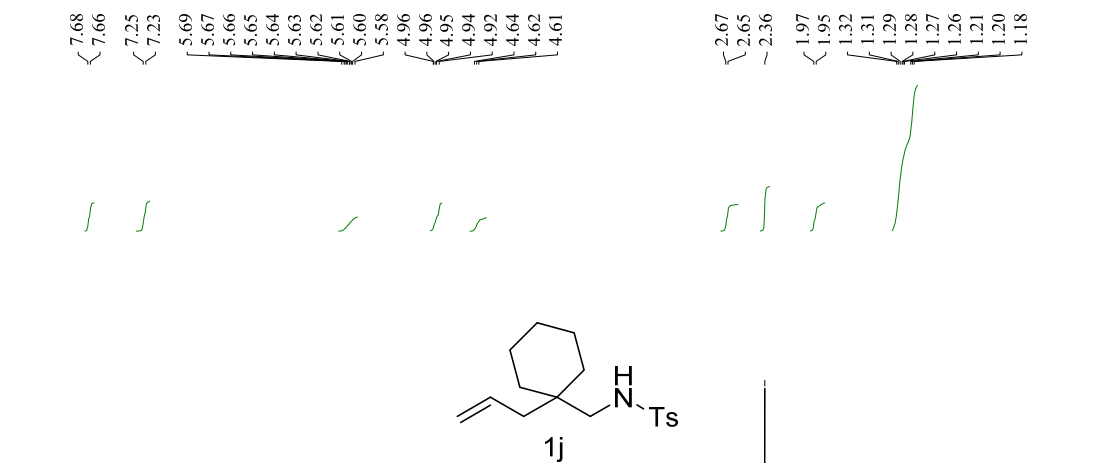
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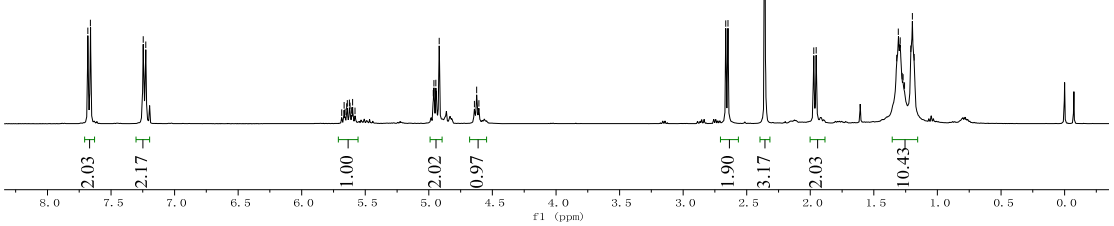
2.67 2.65 2.36 1.97 1.95 1.32 1.31 1.29 1.28 1.27 1.26 1.21 1.20 1.18
H
N
Ts

1j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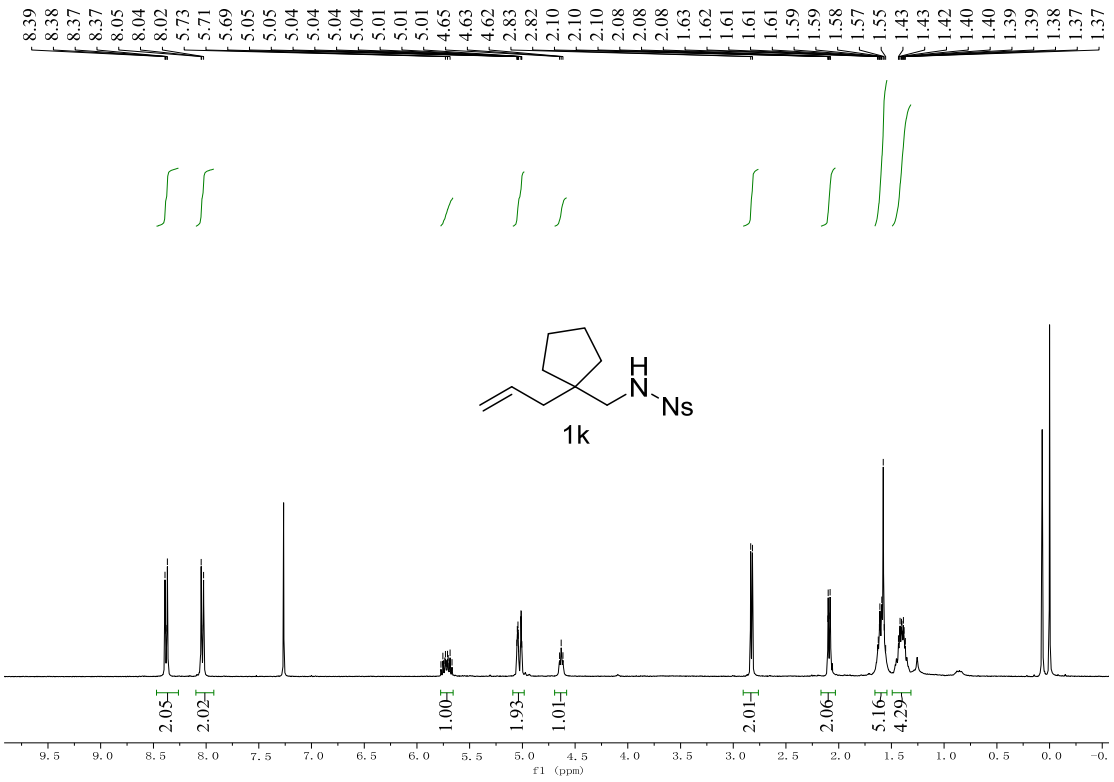
f1 (ppm)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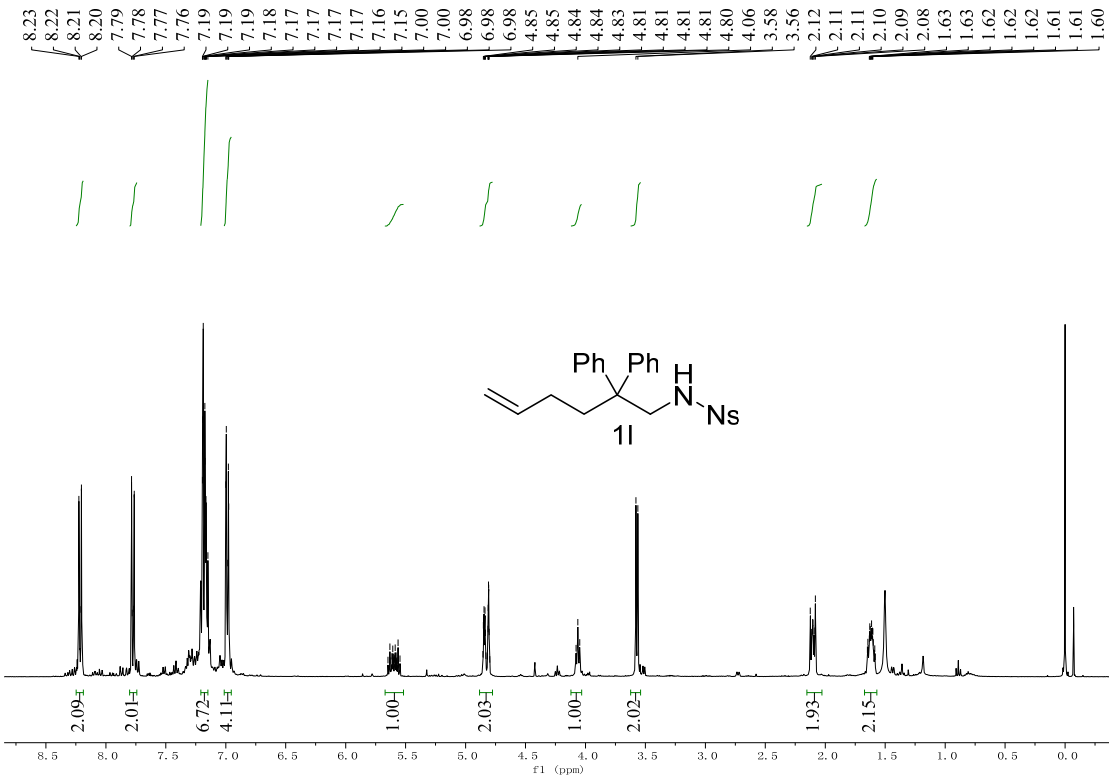
H
N
Ns
1k
2.05 2.02 1.00 1.93 1.01 2.01 2.06 5.16 4.29
f1 (ppm)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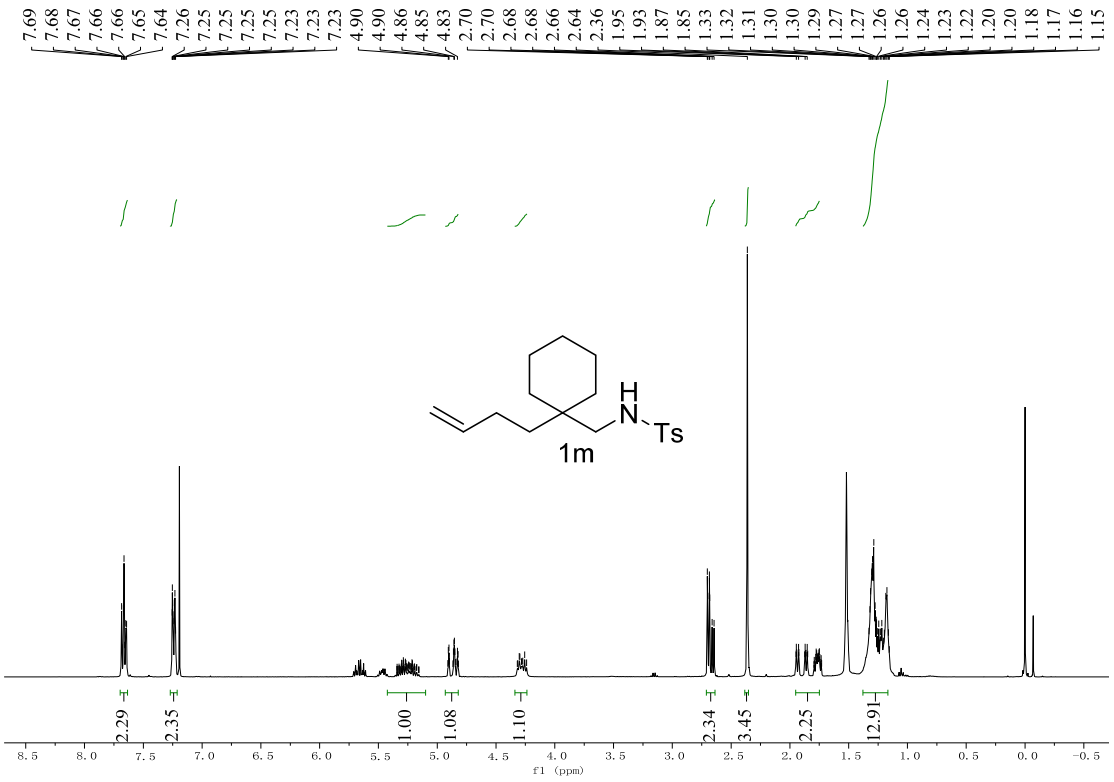
Ph Ph
H
N
Ns
1l
2.09 2.01 6.72 4.11 1.00 2.03 1.00 2.02 1.93 2.15
f1 (ppm)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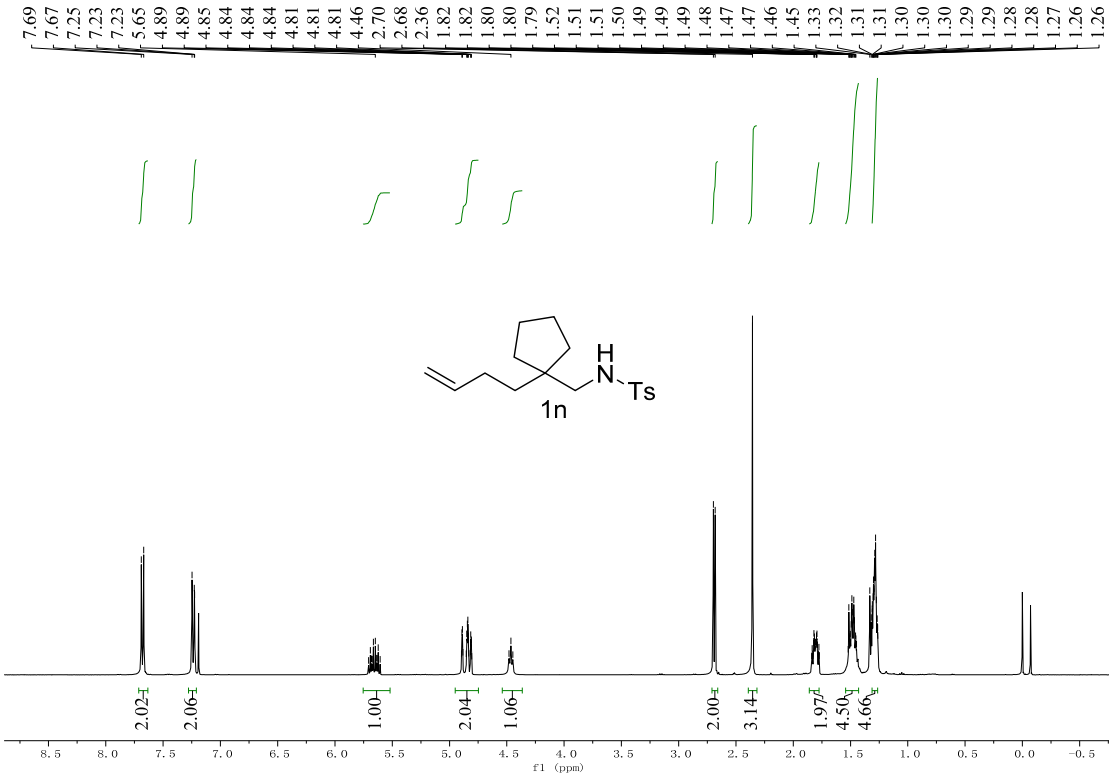
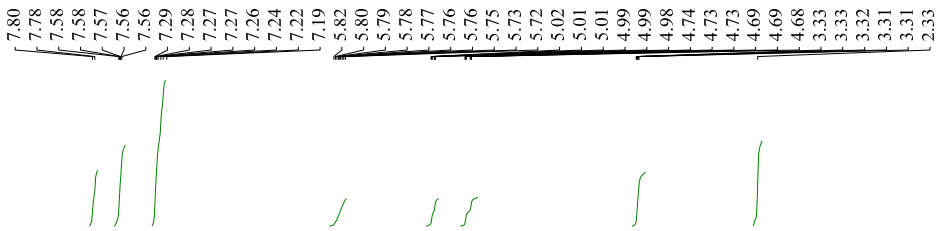
H
N
Ts
1m
2.29 2.35 1.00 1.08 1.10 2.34 3.45 2.25 12.91
f1 (ppm)


7.69 7.67 7.25 7.23 7.23 5.65 4.89 4.89 4.85 4.84 4.84 4.84 4.81 4.81 4.81 4.46 2.70 2.68 2.36 1.82 1.82 1.80 1.80 1.79 1.52 1.51 1.51 1.50 1.49 1.49 1.49 1.48 1.47 1.47 1.46 1.45 1.33 1.32 1.31 1.31 1.30 1.30 1.30 1.29 1.29 1.28 1.28 1.27 1.26 1.26
H
N
Ts
1n
2.02 2.06 1.00 2.04 1.06 2.00 3.14 1.97 4.50 4.66
f1 (ppm)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7.27
7.27
7.26
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7.22
7.19
5.82
5.80
5.79
5.78
5.77
5.76
5.76
5.75
5.73
5.72
5.02
5.01
5.01
4.99
4.99
4.98
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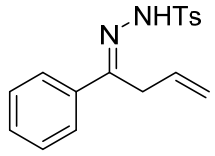
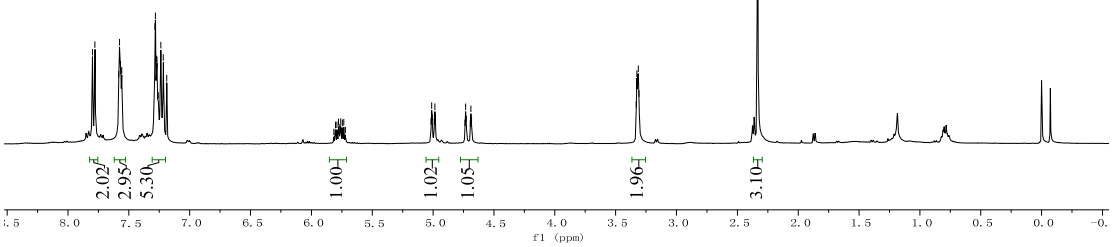
3.33
3.33
3.32
3.31
3.31
2.33


N
NHTs

1o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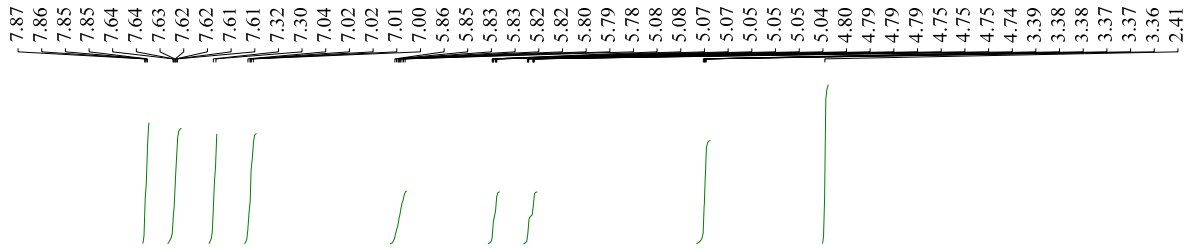
2.95
5.30
1.00
1.02
1.05
1.96
3.10
f1 (ppm)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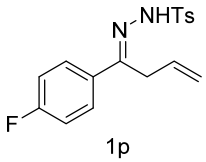
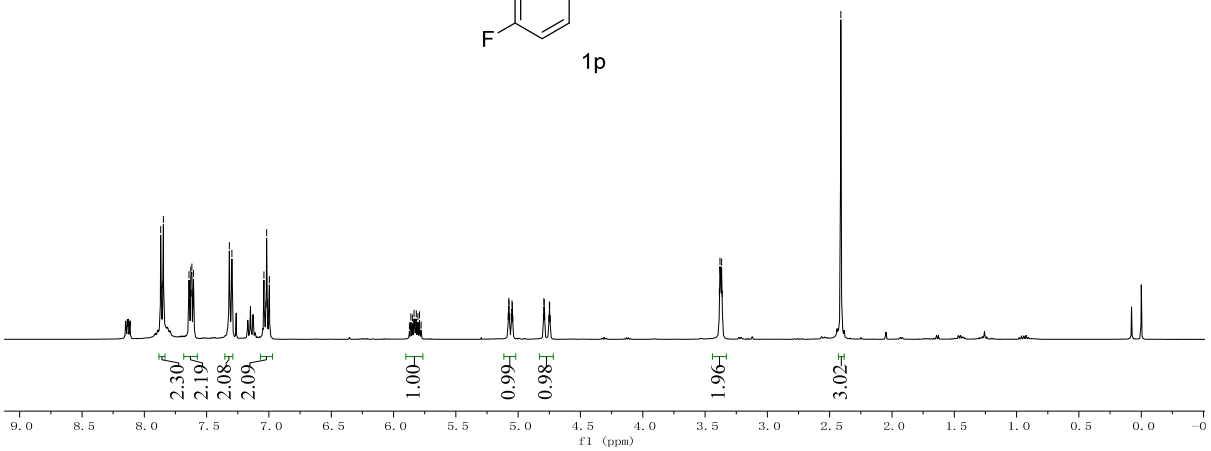
7.85
7.85
7.64
7.64
7.63
7.62
7.62
7.61
7.61
7.32
7.30
7.04
7.02
7.02
7.01
7.00
5.86
5.85
5.83
5.83
5.82
5.82
5.80
5.79
5.78
5.08
5.08
5.07
5.07
5.05
5.05
5.04
4.80
4.79
4.79
4.79
4.75
4.75
4.75
4.74
3.39
3.38
3.38
3.37
3.37
3.36
2.41


N
NHTs
F

1p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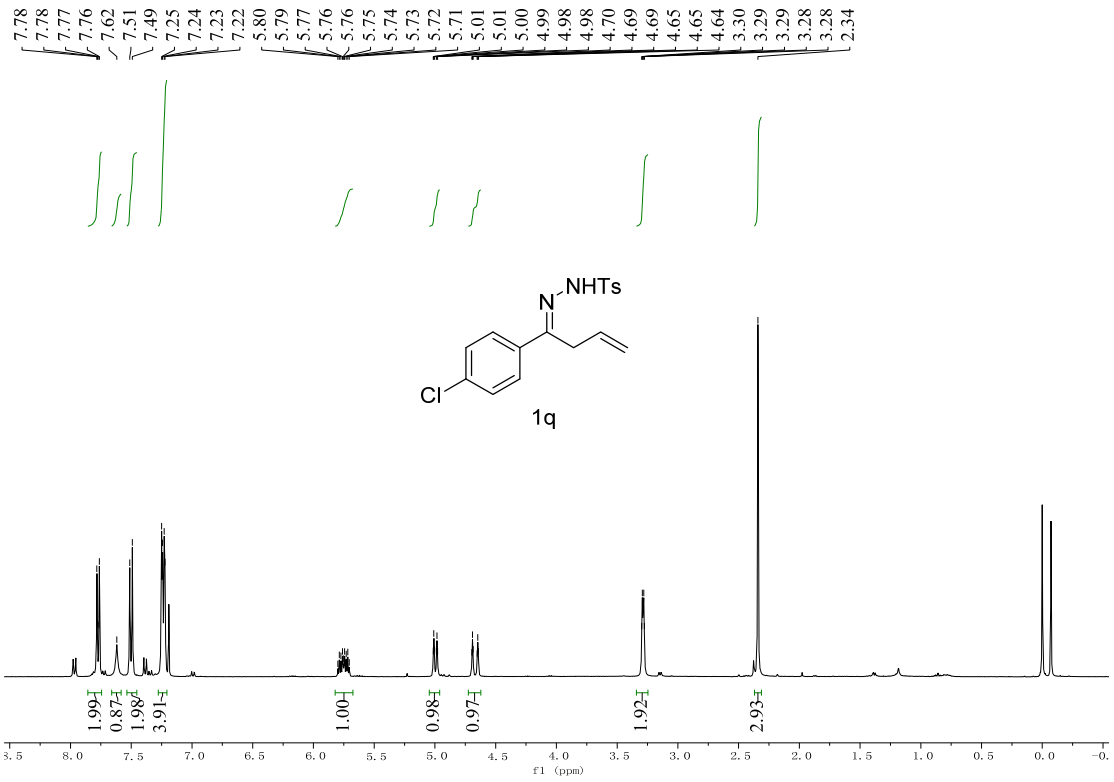
2.08
2.09
1.00
0.99
0.98
1.96
3.02
f1 (ppm)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7.77
7.76
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7.51
7.49
7.25
7.24
7.23
7.22
5.80
5.79
5.77
5.76
5.76
5.75
5.74
5.73
5.72
5.71
5.01
5.01
5.00
4.99
4.98
4.98
4.70
4.69
4.69
4.65
4.65
4.64
3.30
3.29
3.29
3.28
3.28
2.34
NHTs
N
Cl
1q
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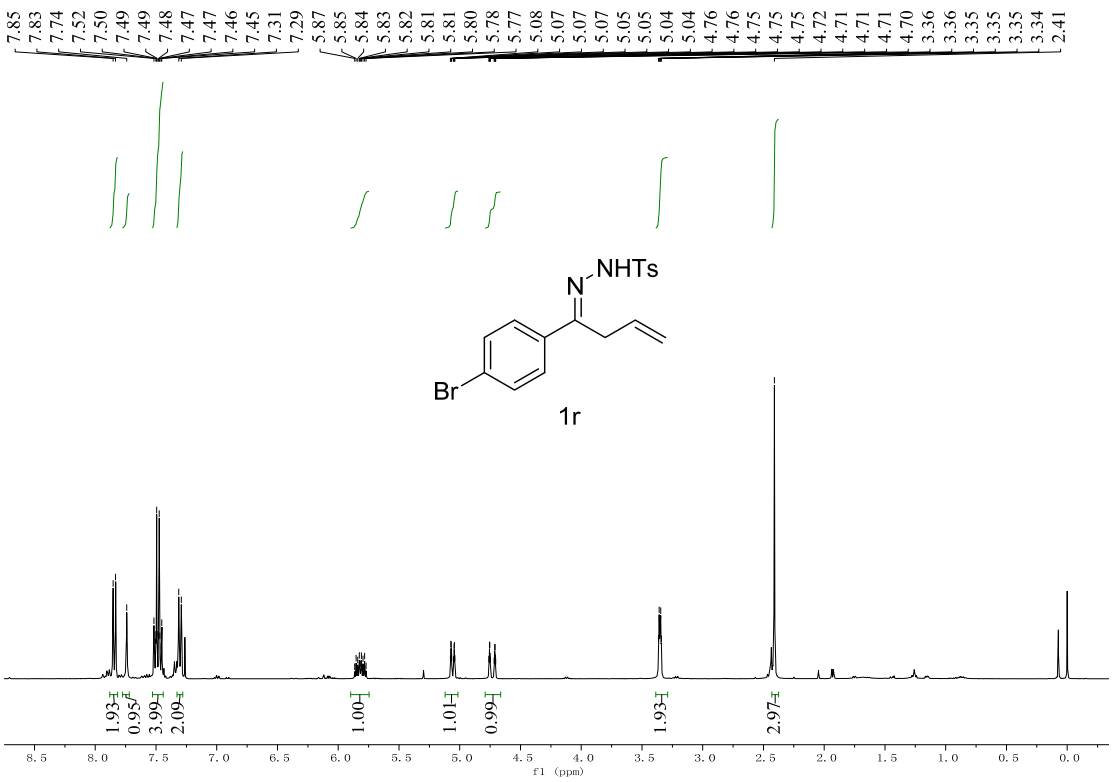
0.87
1.98
3.91
1.00
0.98
0.97
1.92
2.93
f1 (ppm)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7.48
7.47
7.47
7.46
7.45
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7.29
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5.85
5.84
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5.82
5.81
5.81
5.80
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5.05
5.05
5.04
5.04
4.76
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4.75
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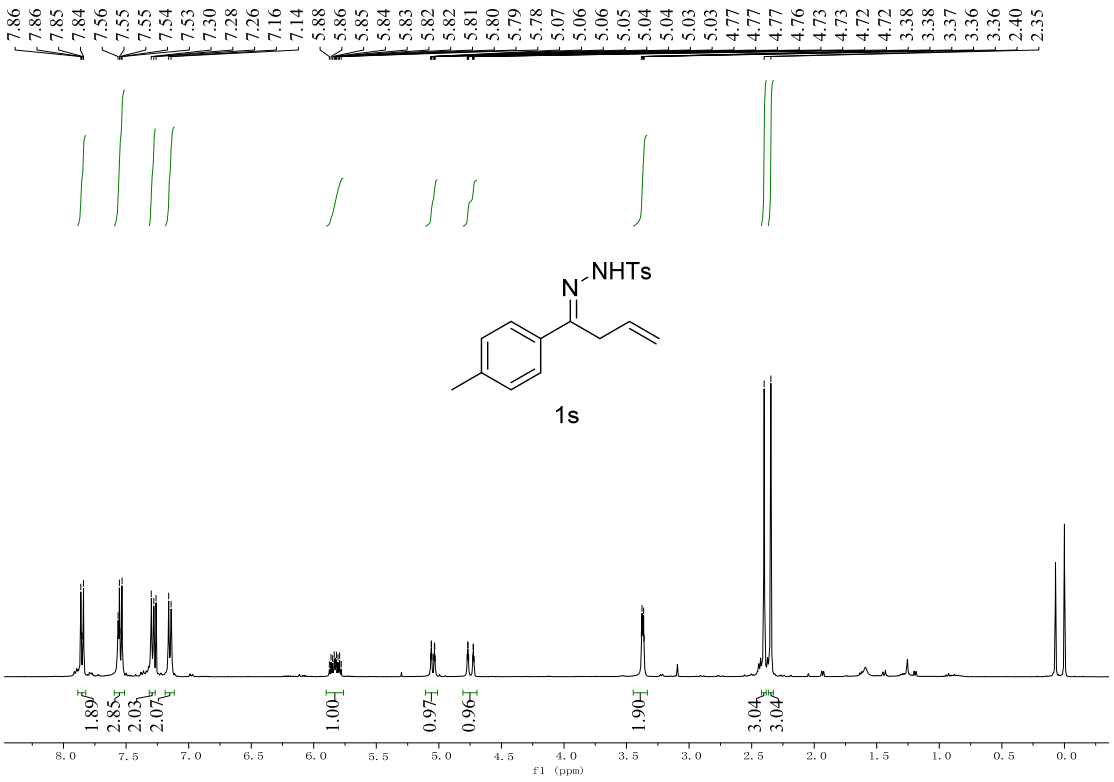
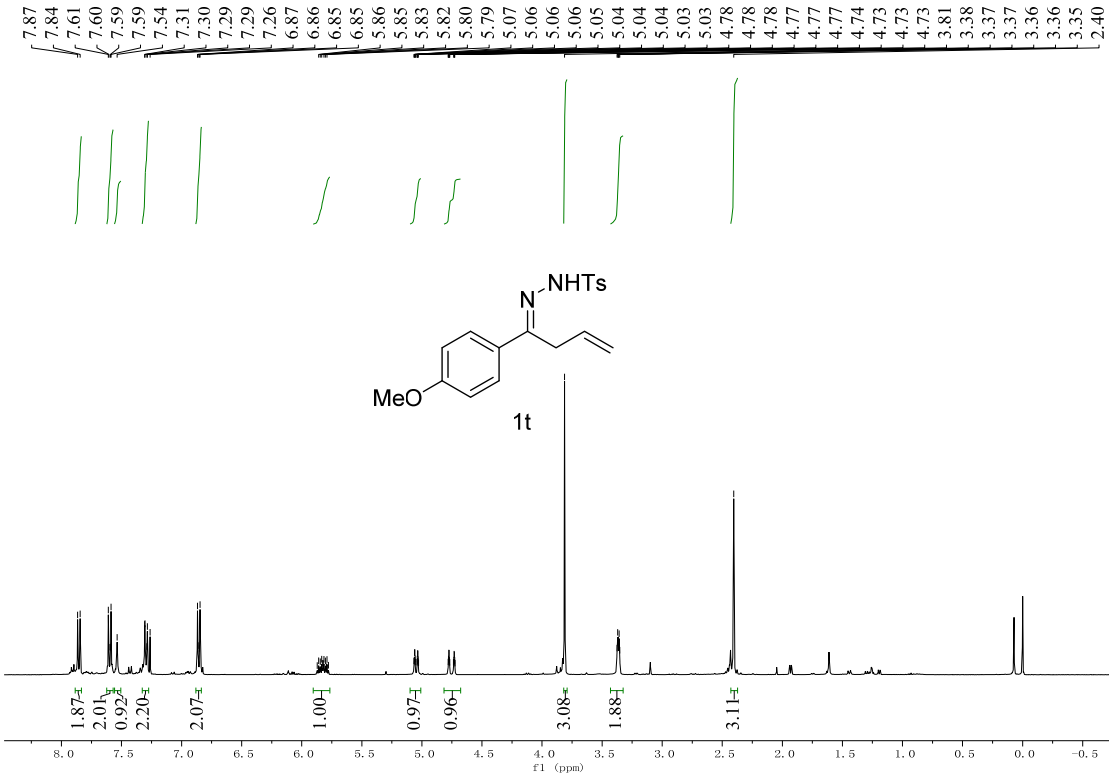
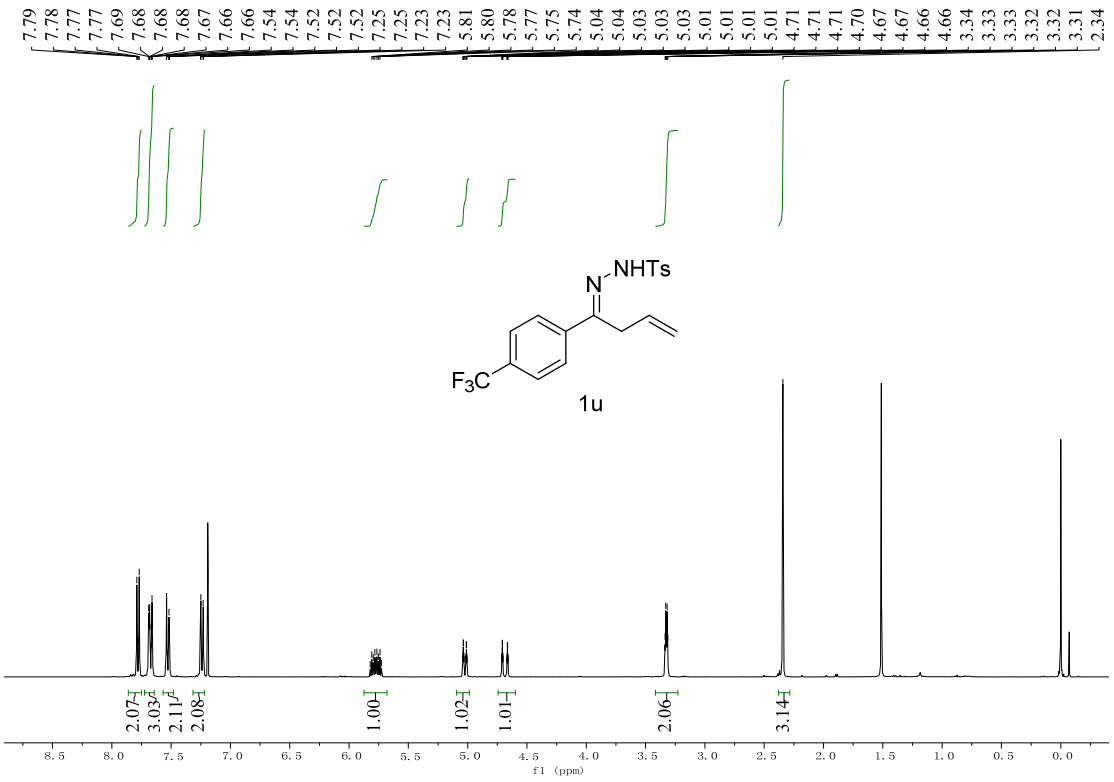
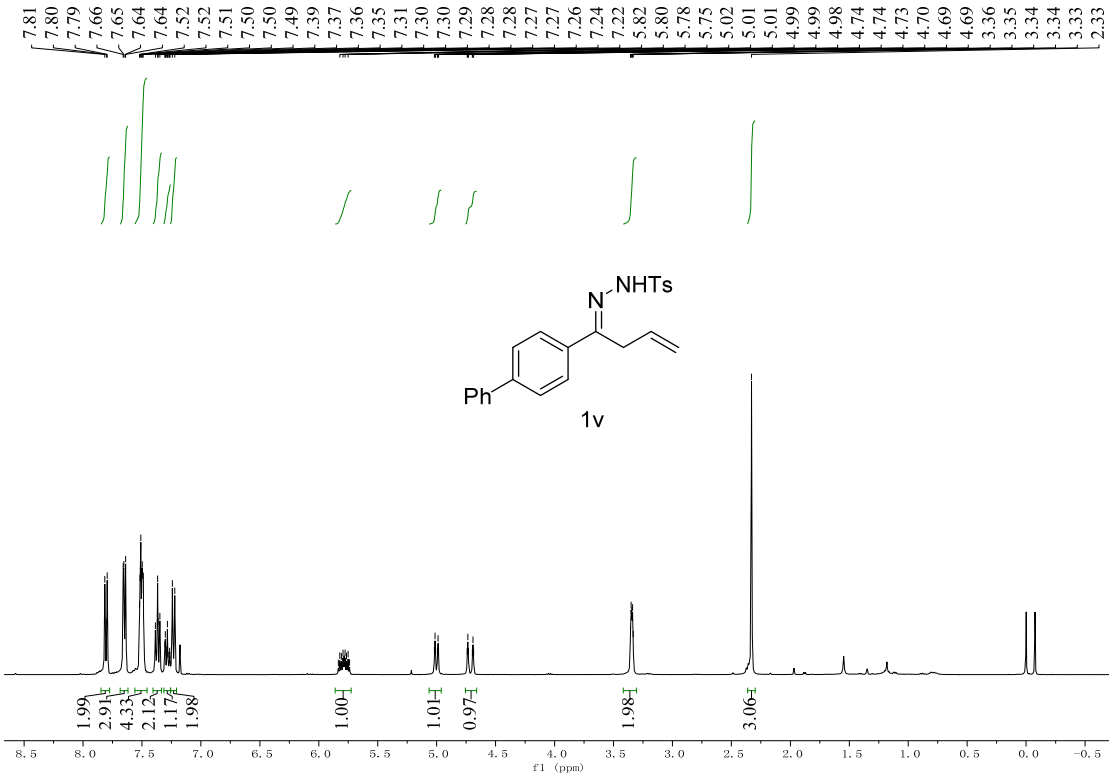
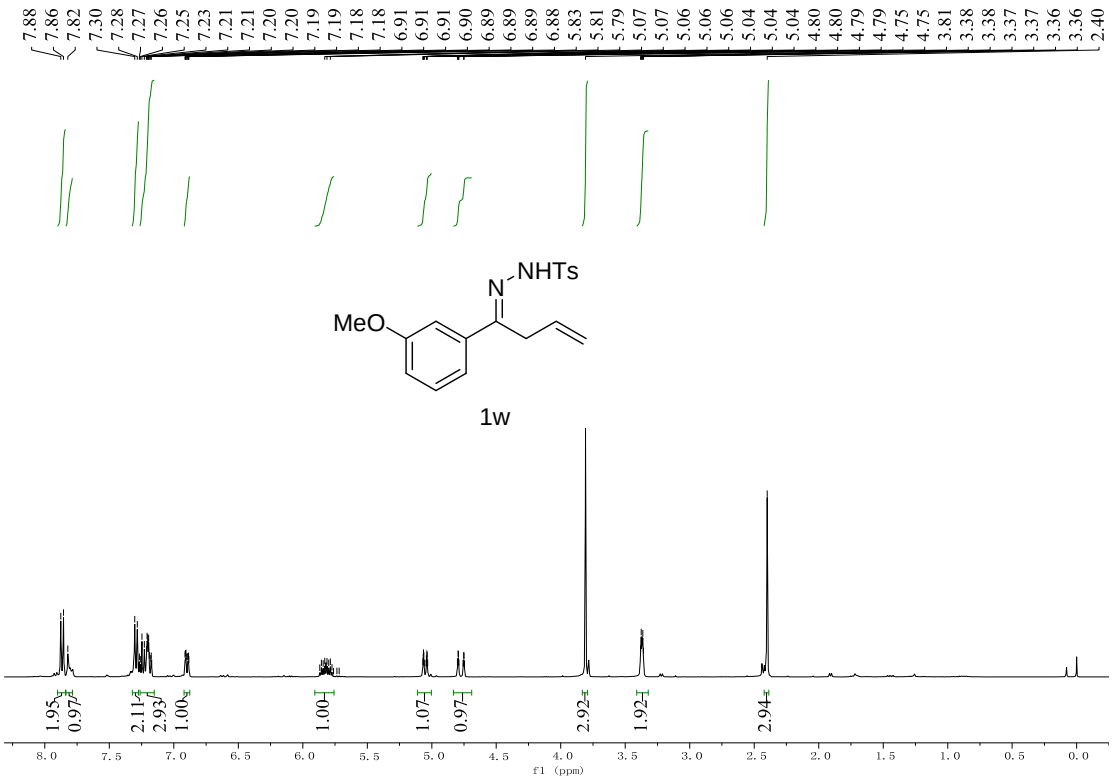
4.75
4.72
4.71
4.71
4.71
4.70
3.36
3.36
3.35
3.35
3.35
3.34
2.41
NHTs
N
Br
1r
1.93
0.95
3.99
2.09
1.00
1.01
0.99
1.93
2.97
f1 (ppm)

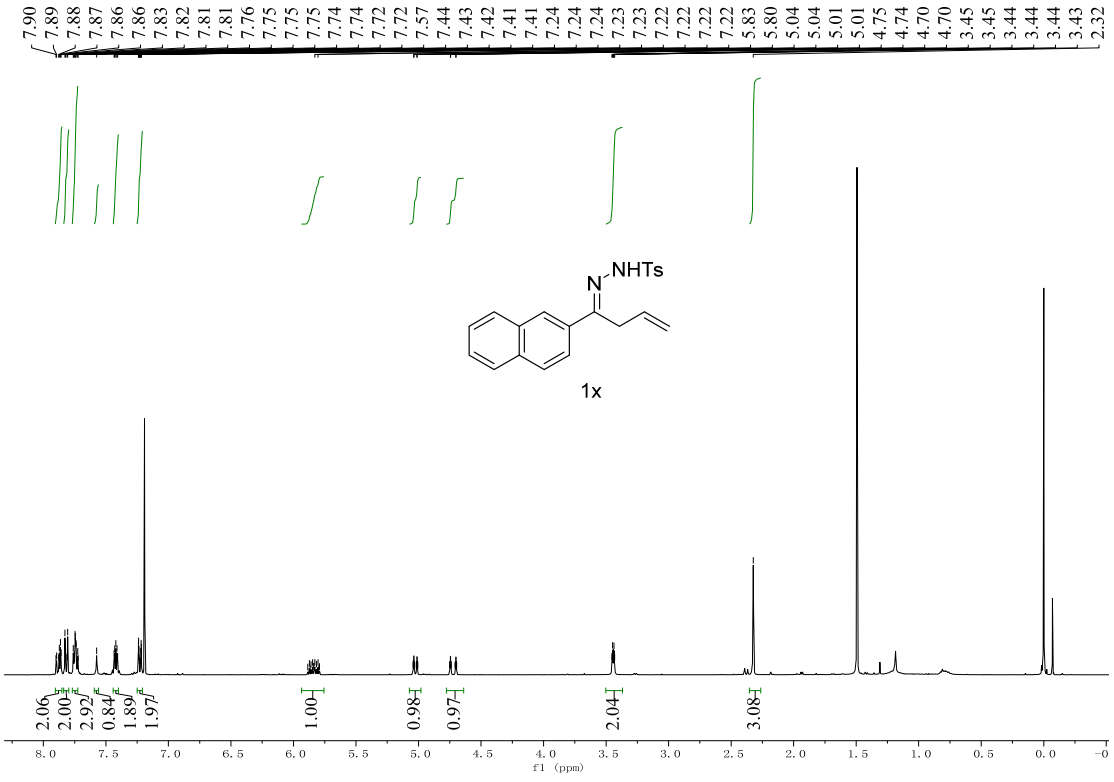

7.86 7.86 7.85 7.84 7.56 7.55 7.55 7.54 7.53 7.30 7.28 7.26 7.16 7.14 5.88 5.86 5.85 5.84 5.83 5.82 5.82 5.81 5.80 5.79 5.78 5.07 5.06 5.06 5.05 5.04 5.04 5.03 5.03 4.77 4.77 4.76 4.73 4.73 4.72 4.72 3.38 3.38 3.37 3.36 3.36 2.40 2.35
N NHTs
1s
1.89 2.85 2.03 2.07 1.00 0.97 0.96 1.90 3.04 3.04
f1 (ppm)

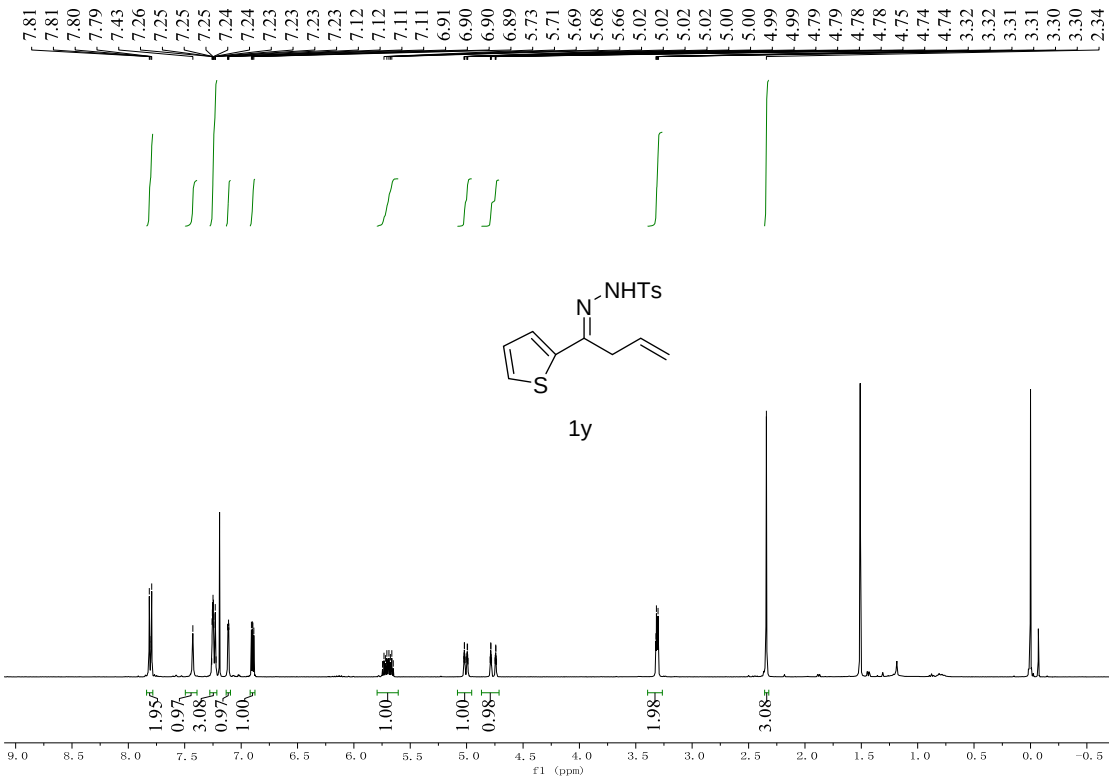

7.87 7.84 7.61 7.60 7.59 7.59 7.54 7.31 7.30 7.29 7.29 7.26 6.87 6.86 6.85 6.85 5.86 5.85 5.83 5.82 5.80 5.79 5.07 5.06 5.06 5.06 5.05 5.04 5.04 5.04 5.03 5.03 4.78 4.78 4.78 4.77 4.77 4.77 4.74 4.73 4.73 3.81 3.38 3.37 3.37 3.36 3.36 3.35 2.40
N NHTs
MeO
1t
1.87 2.01 0.92 2.20 2.07 1.00 0.97 0.96 3.08 1.88 3.11
f1 (ppm)

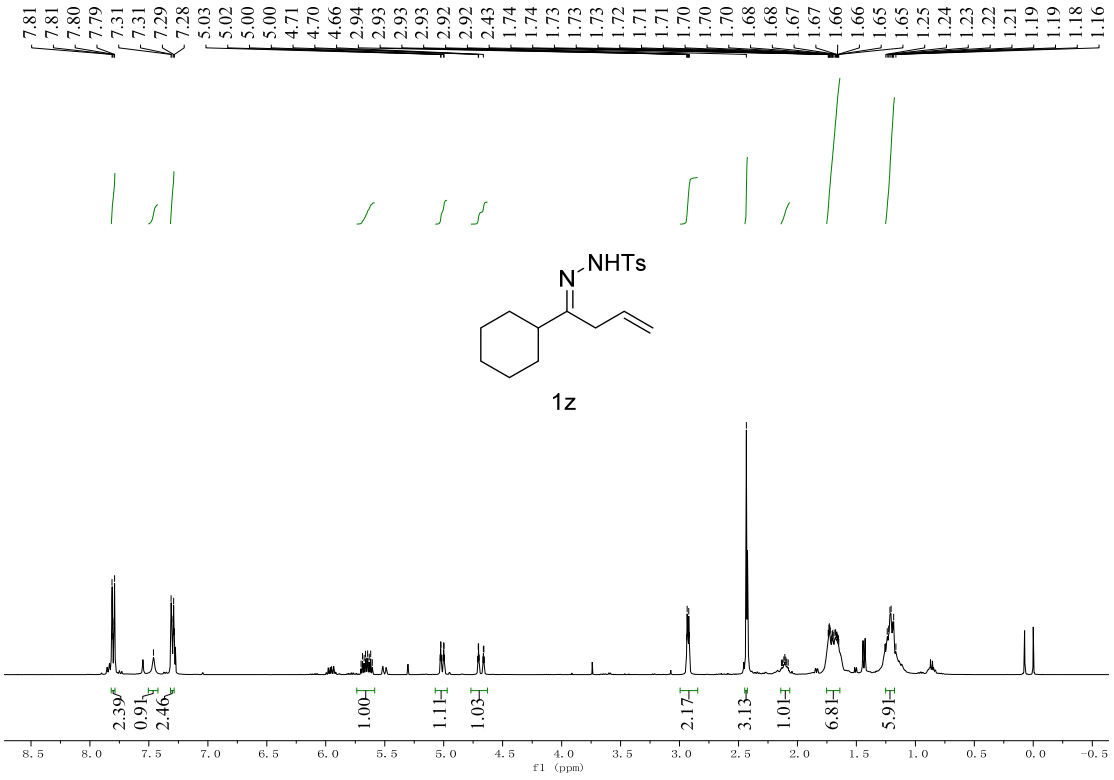

NHTs
N
F3C
1u
f1 (ppm)

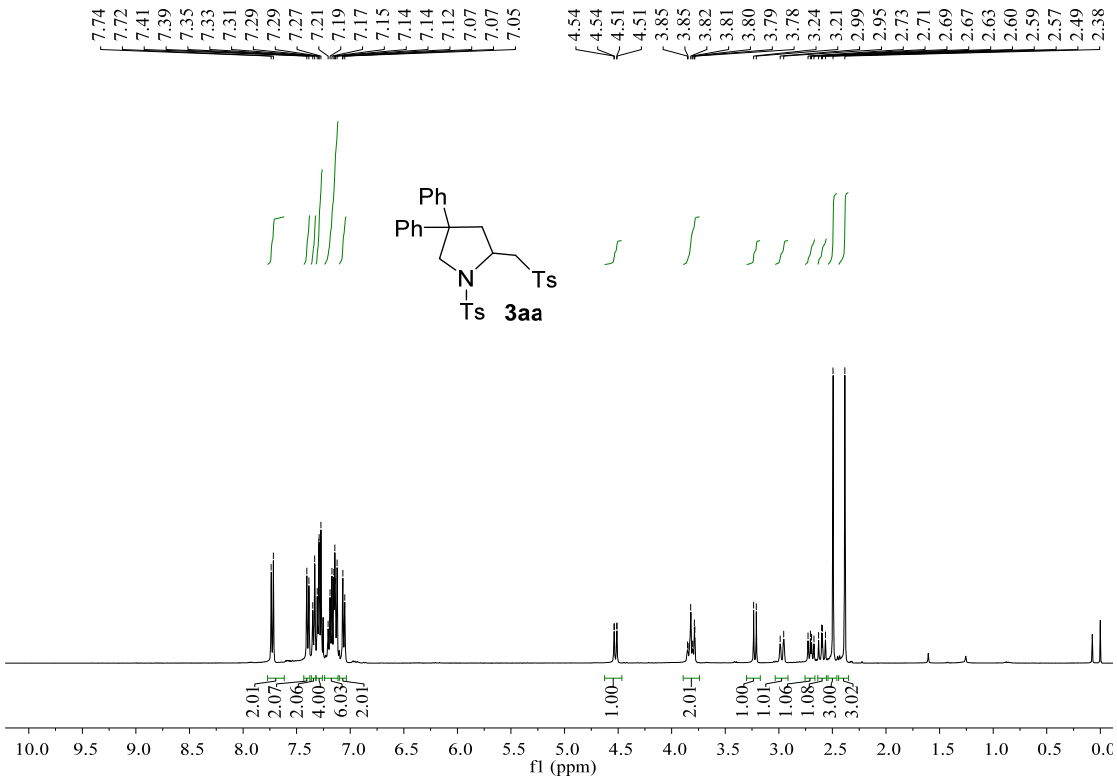

NHTs
N
Ph
1v
f1 (ppm)

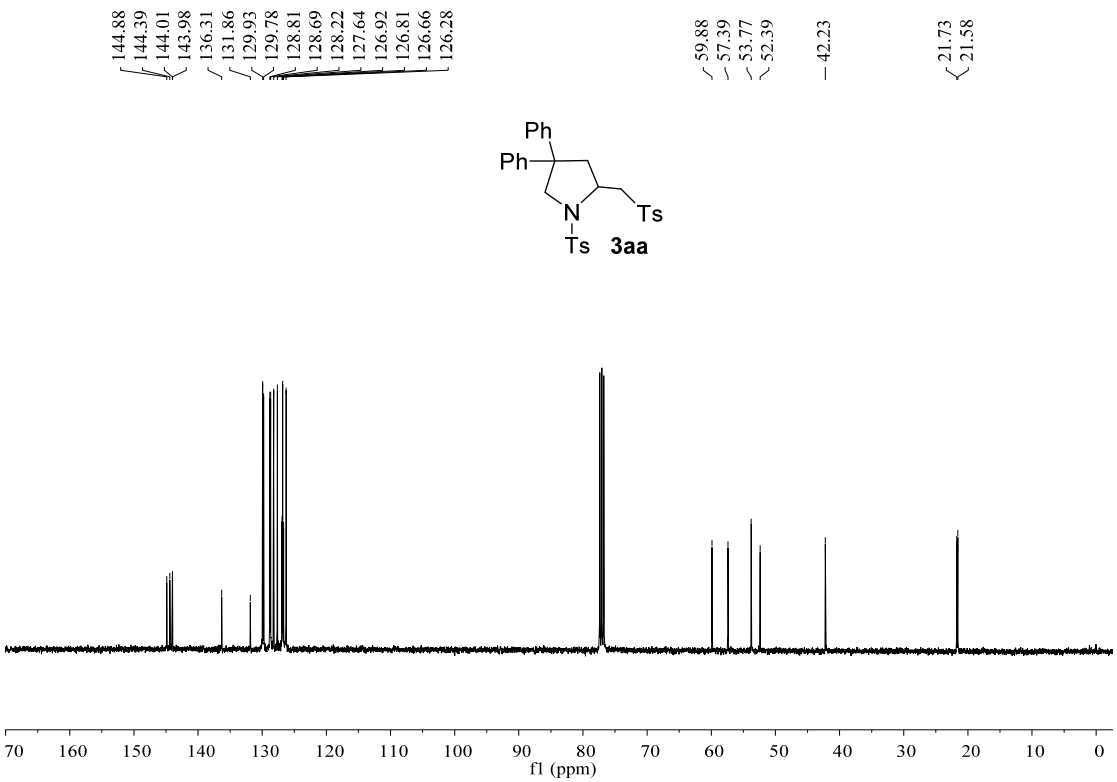

NHTs
N
MeO
1w
f1 (ppm)

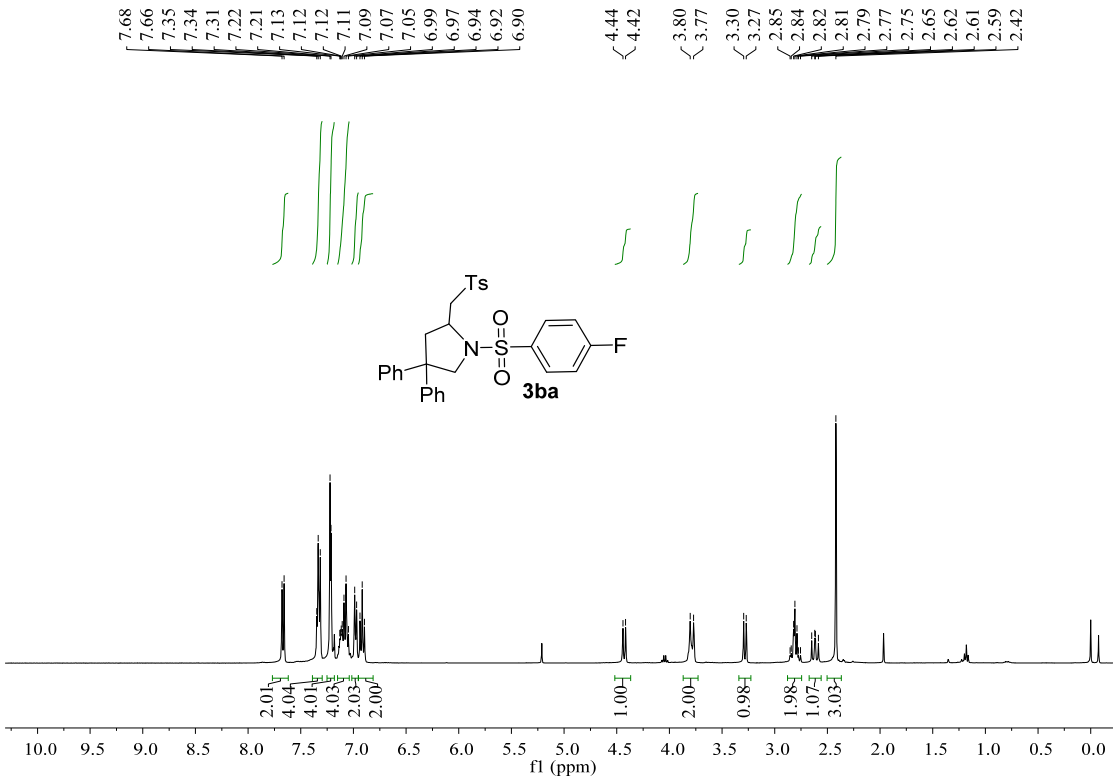

NHTs
N
1x
f1 (ppm)


7.81 7.81 7.80 7.79 7.43 7.26 7.25 7.25 7.25 7.24 7.24 7.23 7.23 7.23 7.23 7.12 7.12 7.11 7.11 6.91 6.90 6.90 6.89 5.73 5.71 5.69 5.68 5.66 5.02 5.02 5.02 5.02 5.00 5.00 4.99 4.99 4.79 4.79 4.78 4.78 4.75 4.74 4.74 3.32 3.32 3.31 3.31 3.30 3.30 2.34
N
NHTs
S
1y
1.95 0.97 3.08 0.97 1.00 1.00 1.00 0.98 1.98 3.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)


7.81 7.81 7.80 7.79 7.31 7.31 7.29 7.28 5.03 5.02 5.00 5.00 4.71 4.70 4.66 2.94 2.93 2.93 2.93 2.92 2.92 2.43 1.74 1.74 1.73 1.73 1.73 1.72 1.71 1.71 1.70 1.70 1.70 1.68 1.68 1.67 1.67 1.66 1.66 1.65 1.65 1.25 1.24 1.23 1.22 1.21 1.19 1.19 1.18 1.16
N
NHTs
1z
2.39 0.91 2.46 1.00 1.11 1.03 2.17 3.13 1.01 6.81 5.91
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)


7.74 7.72 7.41 7.39 7.35 7.33 7.31 7.29 7.29 7.27 7.21 7.19 7.17 7.15 7.14 7.14 7.12 7.07 7.07 7.05
4.54 4.54 4.51 4.51 3.85 3.85 3.82 3.81 3.80 3.79 3.78 3.24 3.21 2.99 2.95 2.73 2.71 2.69 2.67 2.63 2.60 2.59 2.57 2.49 2.38
Ph
Ph
N
Ts
Ts
Ts 3aa
2.01 2.07 2.06 4.00 6.03 2.01 1.00 2.01 1.00 1.01 1.06 1.08 3.00 3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


144.88 144.39 144.01 143.98 136.31 131.86 129.93 129.78 128.81 128.69 128.22 127.64 126.92 126.81 126.66 126.28
59.88 57.39 53.77 52.39 42.23 21.73 21.58
Ph
Ph
N
Ts
Ts
Ts 3aa
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.12
7.11
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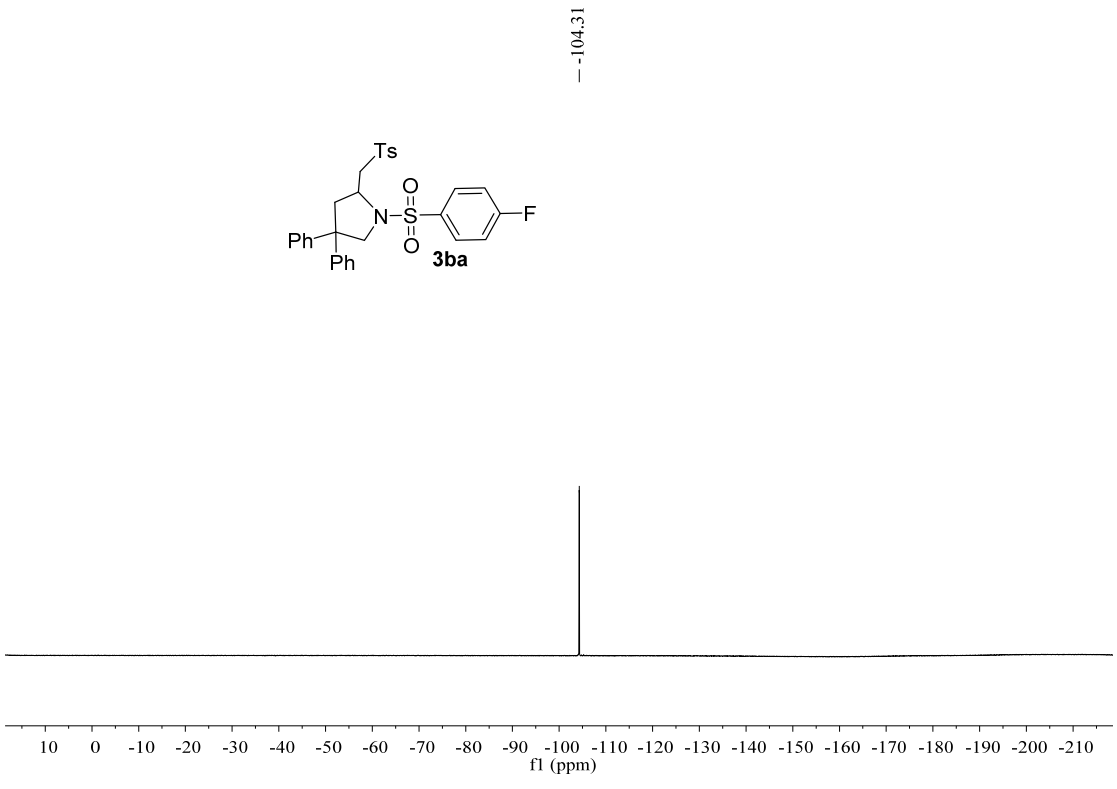
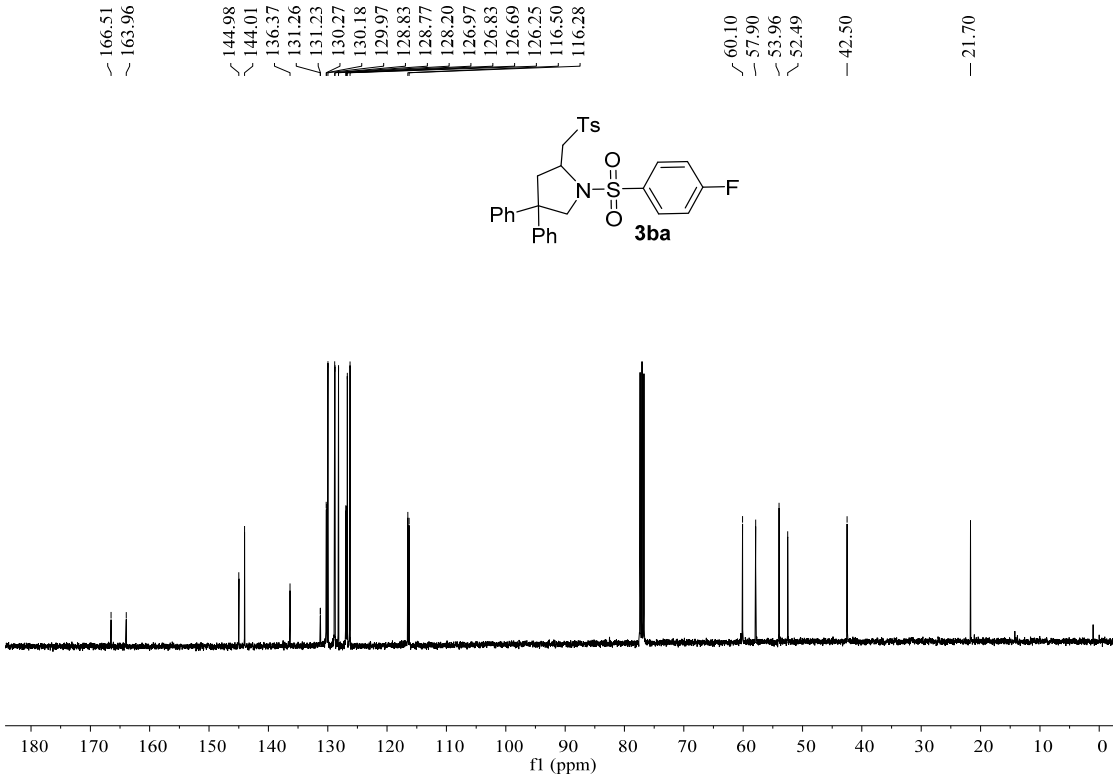
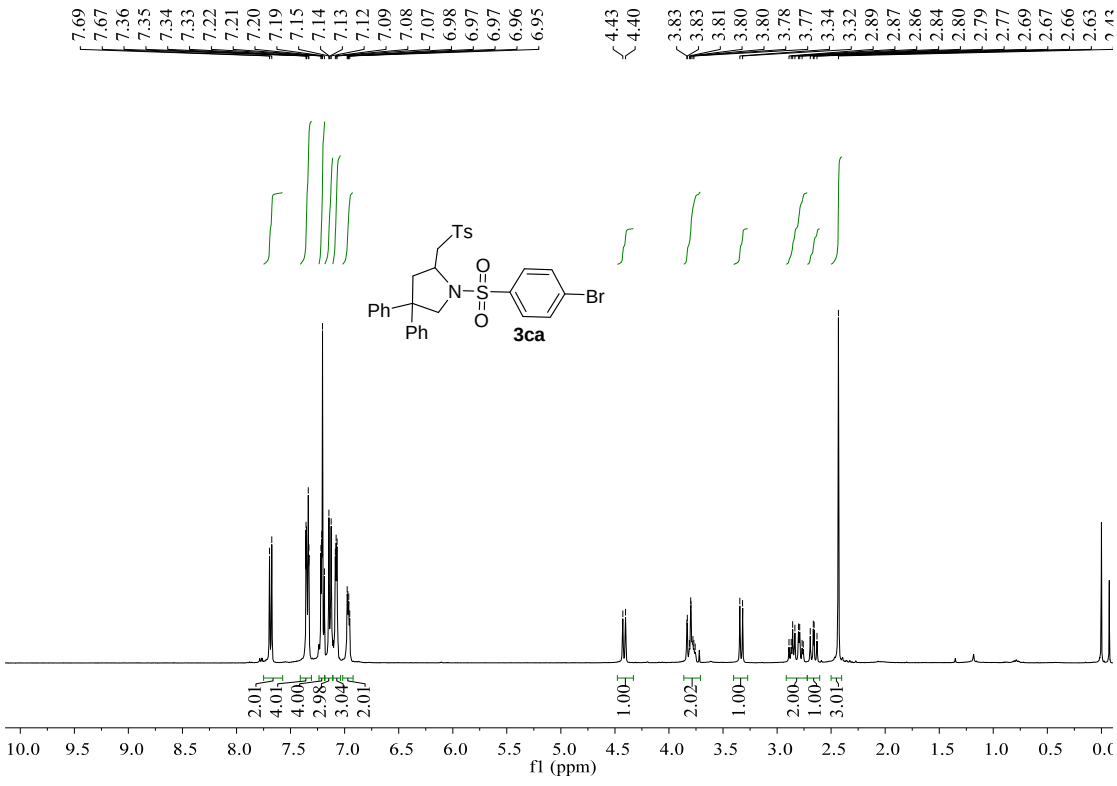
7.07
7.05
6.99
6.97
6.94
6.92
6.90
4.44
4.42
3.80
3.77
3.30
3.27
2.85
2.84
2.82
2.81
2.79
2.77
2.75
2.65
2.62
2.61
2.59
2.42
Ts
O
N
S
O
F
Ph
Ph
3ba
2.01
4.04
4.01
4.03
2.03
2.00
1.00
2.00
0.98
1.98
1.07
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-104.31
Ts
O
N
S
O
F
Ph
Ph
3ba
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


166.51
163.96
144.98
144.01
136.37
131.26
131.23
130.27
130.18
129.97
128.83
128.77
128.20
126.97
126.83
126.69
126.25
116.50
116.28
60.10
57.90
53.96
52.49
42.50
21.70
Ts
O
N
S
O
F
Ph
Ph
3ba
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.67
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7.33
7.22
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7.20
7.19
7.15
7.14
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7.12
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6.96
6.95
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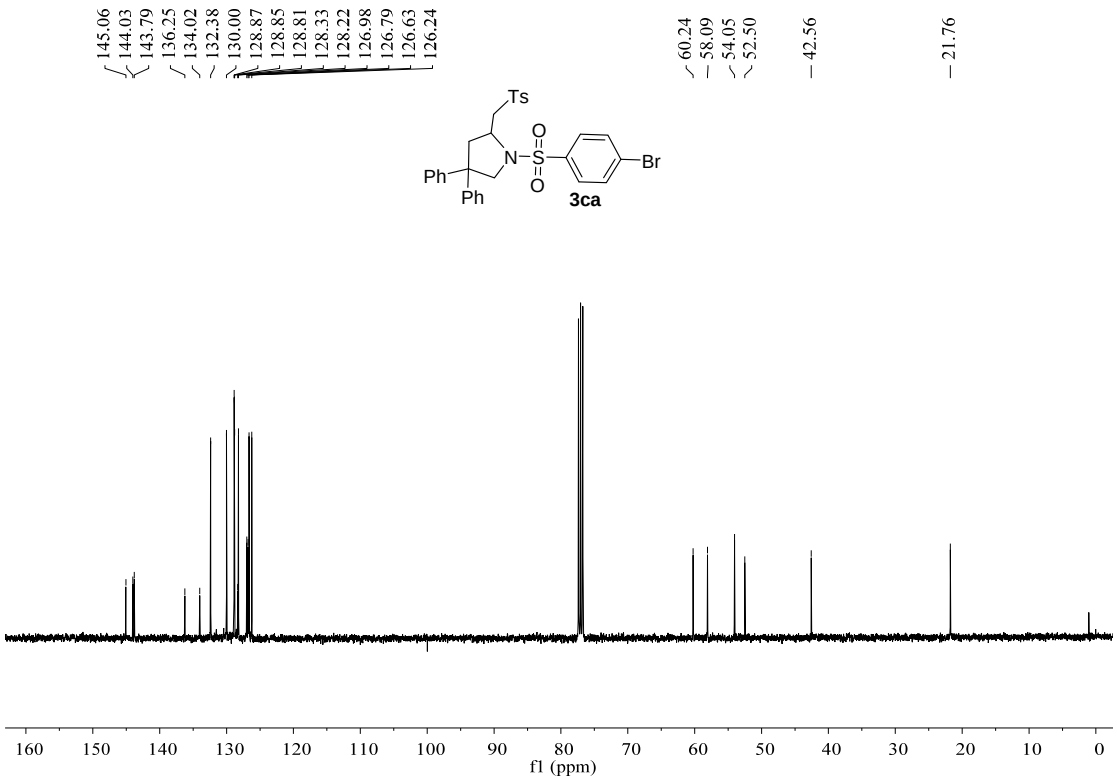
2.87
2.86
2.84
2.80
2.79
2.77
2.69
2.67
2.66
2.63
Ts
O
N
S
O
Br
Ph
Ph
3ca
2.01
4.01
4.00
2.98
3.04
2.01
1.00
2.02
1.00
2.00
1.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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144.03
143.79
136.25
134.02
132.38
130.00
128.87
128.85
128.81
128.33
128.22
126.98
126.79
126.63
126.24
60.24
58.09
54.05
52.50
42.56
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N
S
O
Br
Ph
Ph
3ca
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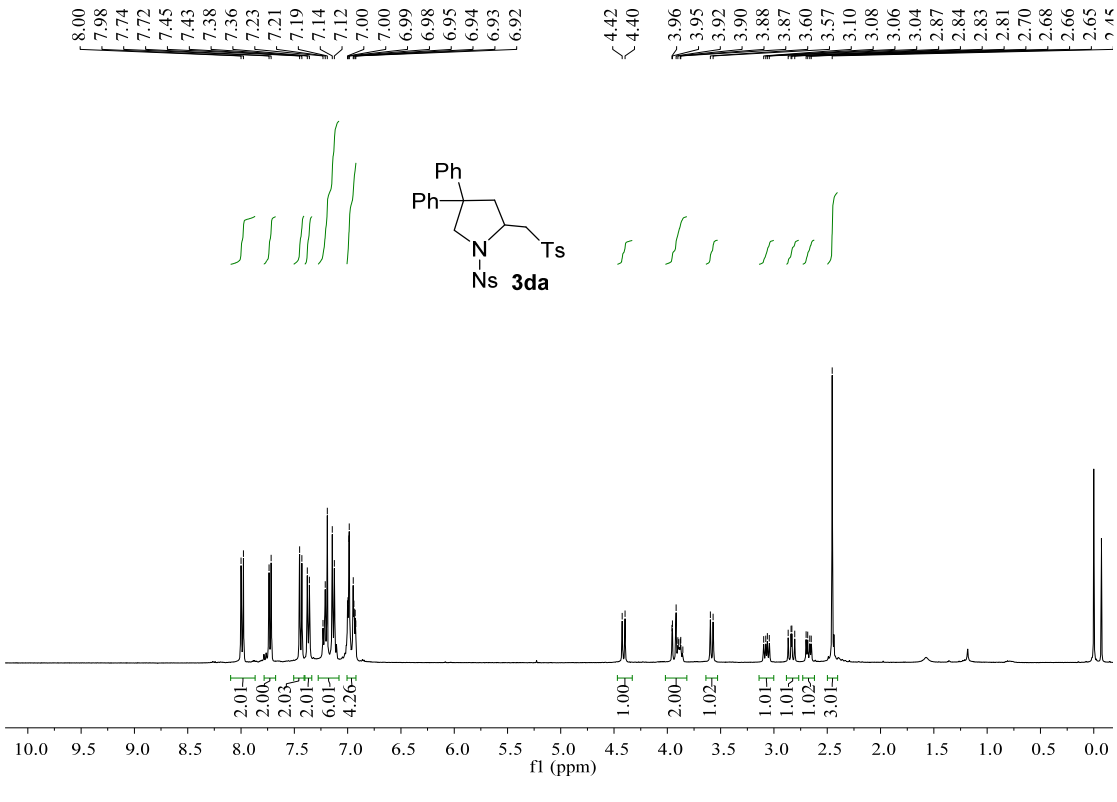
f1 (ppm)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7.19
7.14
7.12
7.00
7.00
6.99
6.98
6.95
6.94
6.93
6.92
4.42
4.40
3.96
3.95
3.92
3.90
3.88
3.87
3.60
3.57
3.10
3.08
3.06
3.04
2.87
2.84
2.83
2.81
2.70
2.68
2.66
2.65
Ph
Ph
N
Ts
Ns
3da
2.01
2.00
2.03
2.01
6.01
4.26
1.00
2.00
1.02
1.01
1.01
1.02
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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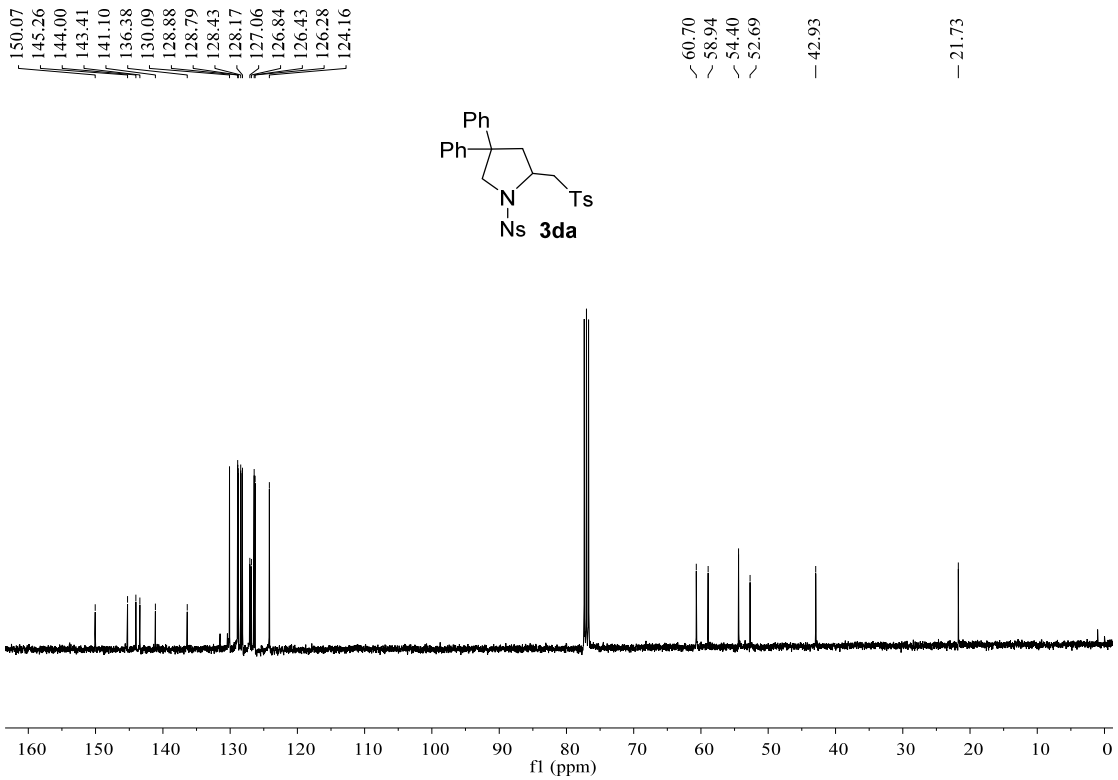
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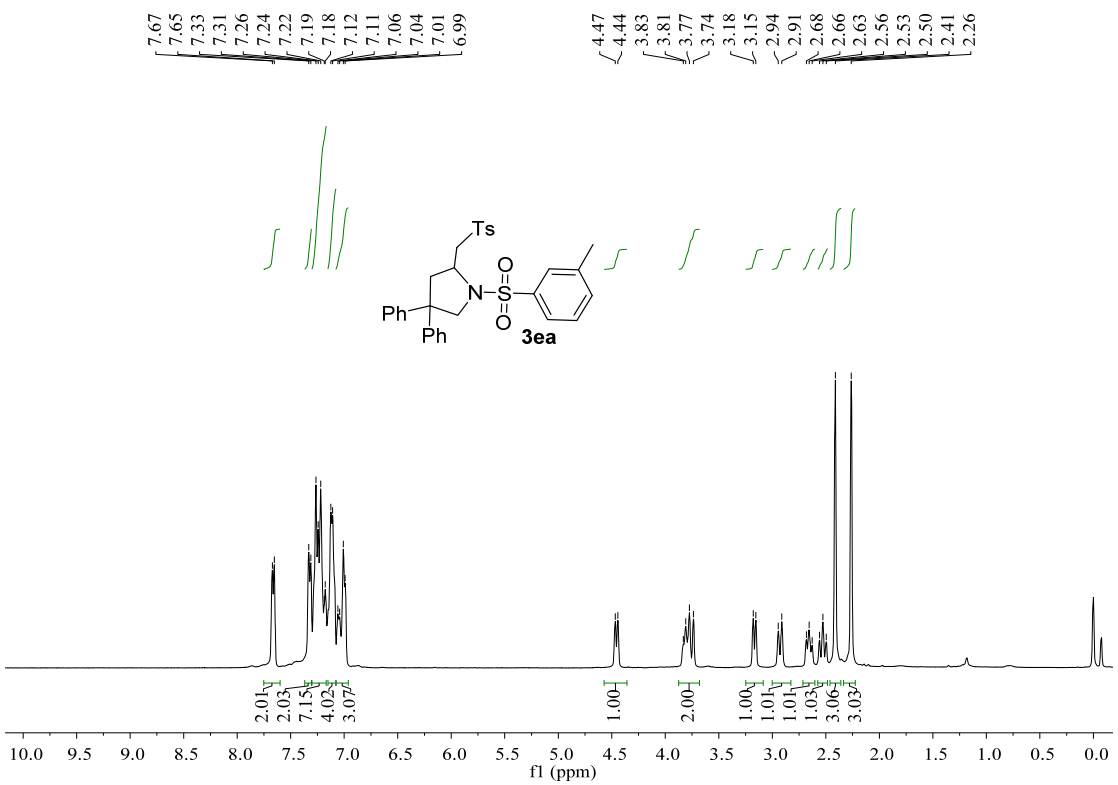
126.43
126.28
124.16
60.70
58.94
54.40
52.69
42.93
21.73
Ph
Ph
N
Ts
Ns
3da
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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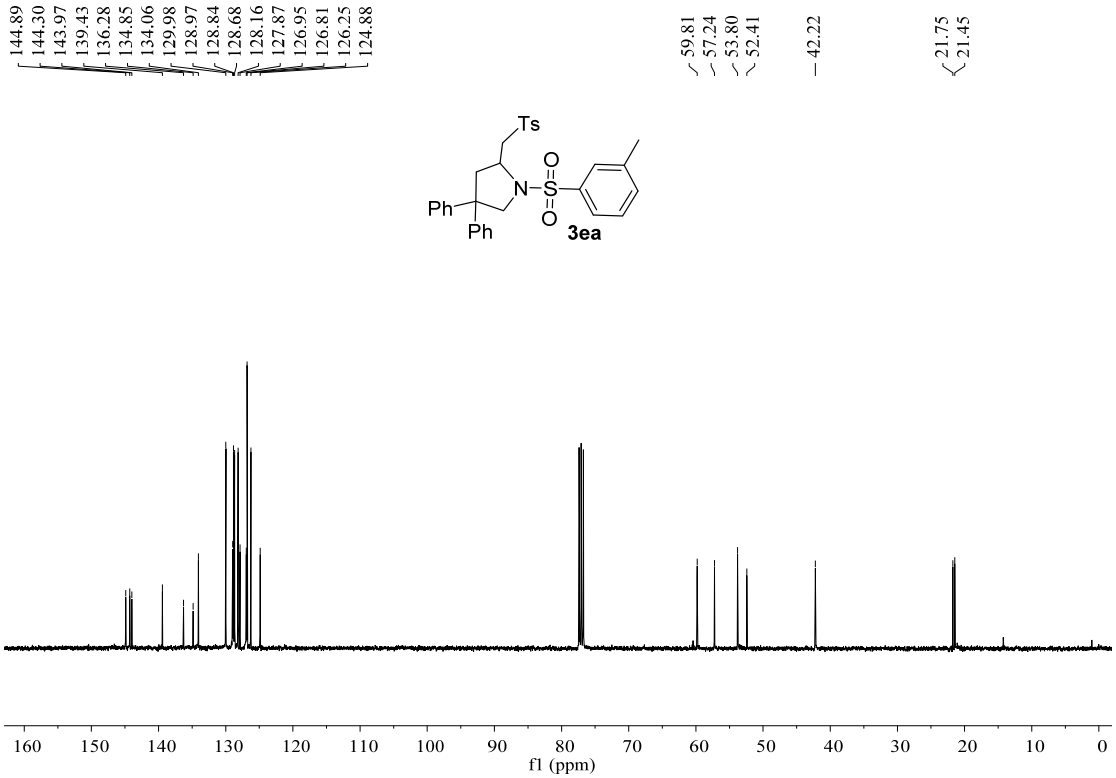
6.99
4.47
4.44
3.83
3.81
3.77
3.74
3.18
3.15
2.94
2.91
2.68
2.66
2.63
2.56
2.53
2.50
2.41
2.26
Ts
O
N
S
O
Ph
Ph
3ea
2.01
2.03
7.15
4.02
3.07
1.00
2.00
1.00
1.01
1.01
1.03
3.06
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.95
126.81
126.25
124.88
59.81
57.24
53.80
52.41
42.22
21.75
21.45
Ts
Ph
Ph
N
S
O
O
3ea
160
150
140
130
120
110
100
90
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50
40
30
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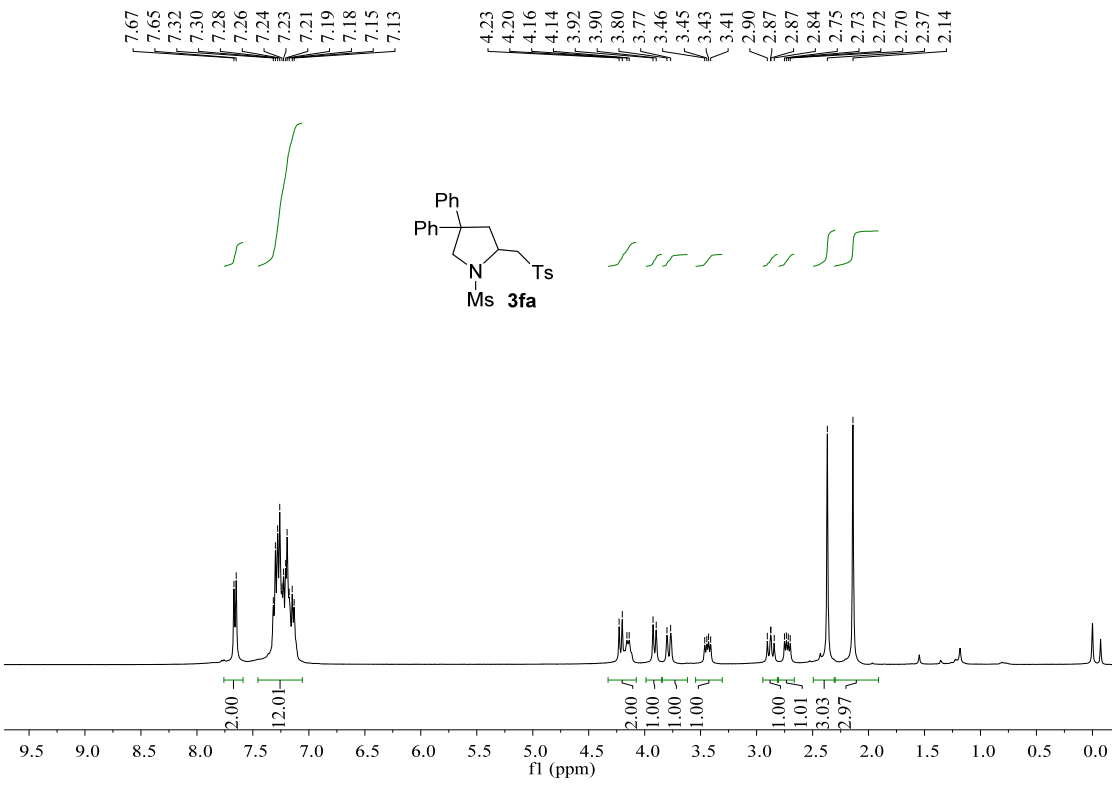
10
0
f1 (ppm)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7.13
4.23
4.20
4.16
4.14
3.92
3.90
3.80
3.77
3.46
3.45
3.43
3.41
2.90
2.87
2.87
2.84
2.75
2.73
2.72
2.70
2.37
2.14
Ph
Ph
N
Ts
Ms
3fa
2.00
12.01
2.00
1.00
1.00
1.00
1.00
1.01
3.03
2.97
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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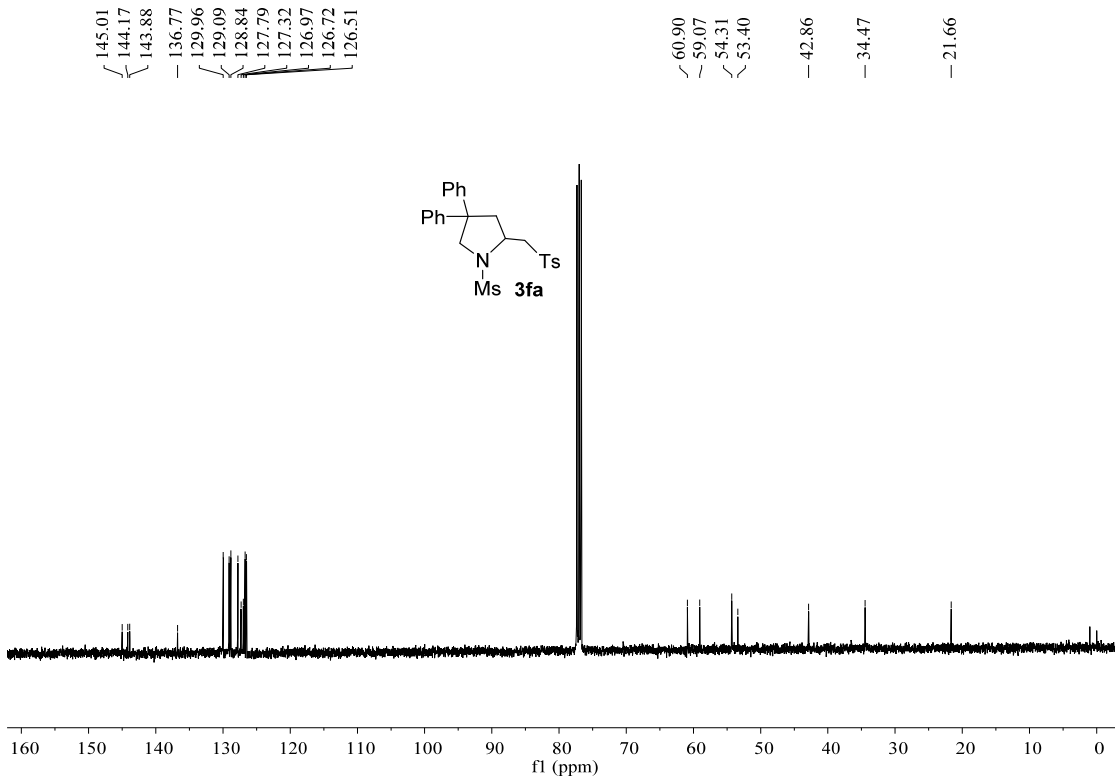
0.0
f1 (ppm)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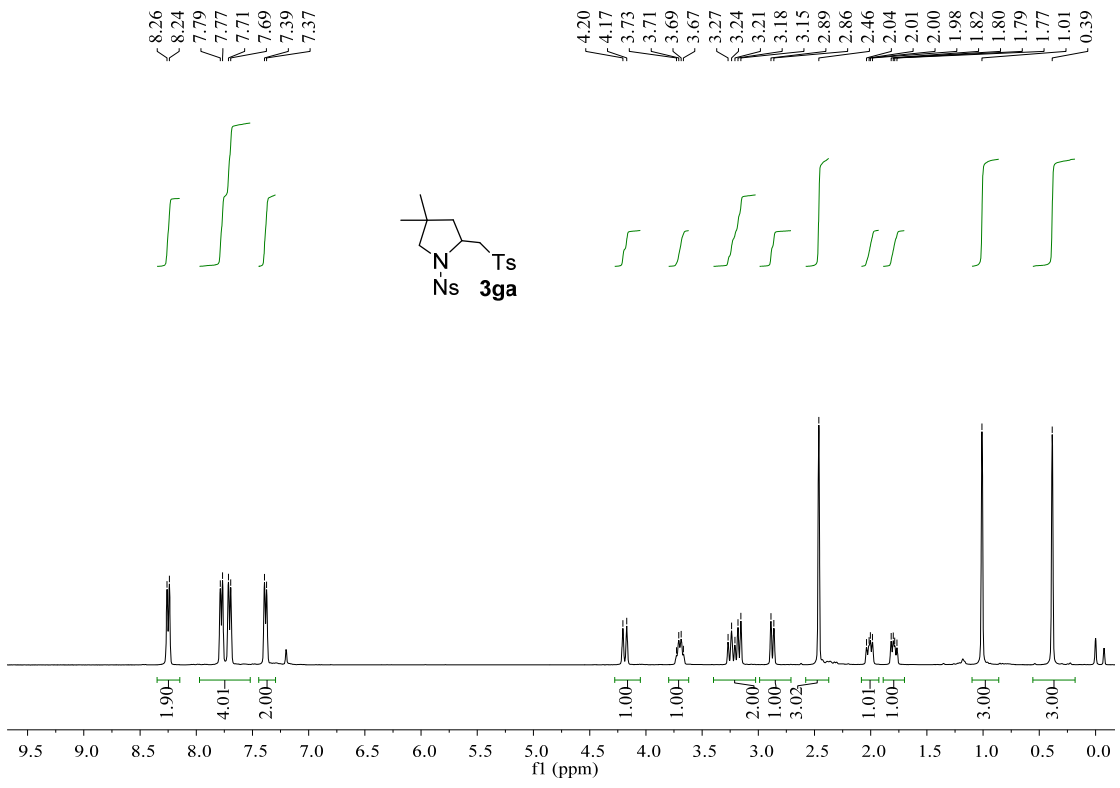
129.09
128.84
127.79
127.32
126.97
126.72
126.51
60.90
59.07
54.31
53.40
42.86
34.47
21.66
Ph
Ph
N
Ms
Ts
3fa
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.69
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7.37
4.20
4.17
3.73
3.71
3.69
3.67
3.27
3.24
3.21
3.18
3.15
2.89
2.86
2.46
2.04
2.01
2.00
1.98
1.82
1.80
1.79
1.77
1.01
0.39
N
Ns
Ts
3ga
1.90
4.01
2.00
1.00
1.00
2.00
1.00
3.02
1.01
1.00
3.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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1.0
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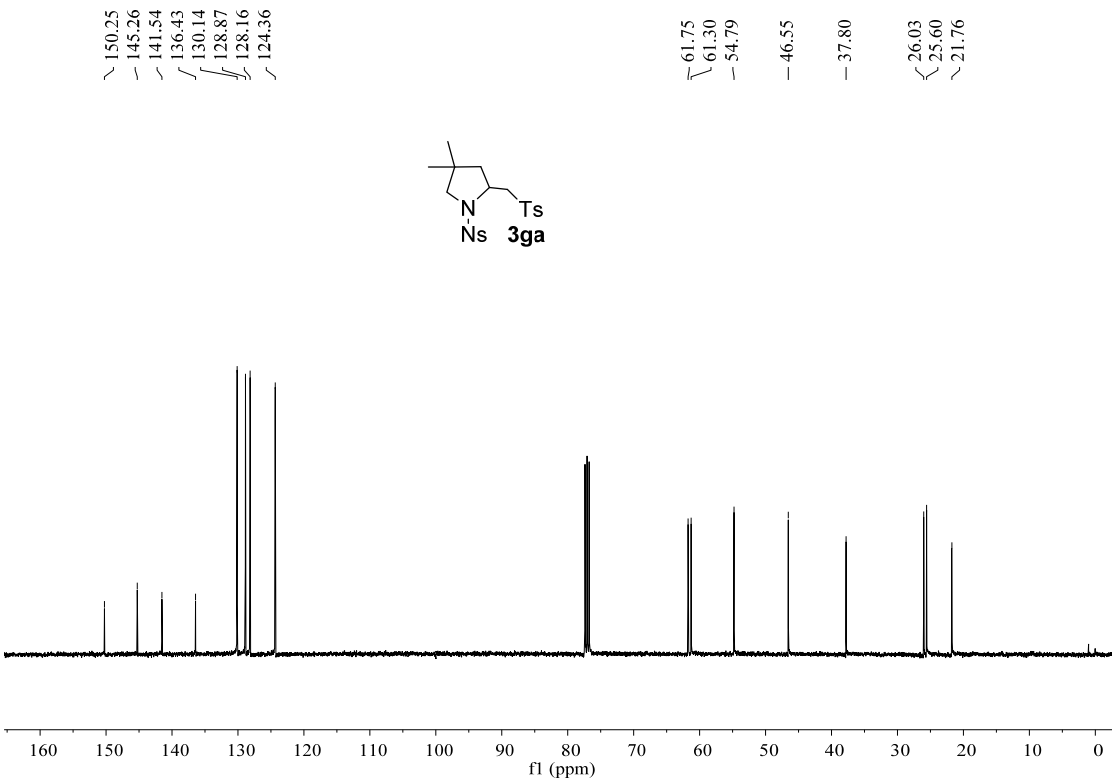
0.0
f1 (ppm)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128.87
128.16
124.36
61.75
61.30
54.79
46.55
37.80
26.03
25.60
21.76
Ts
N
Ns
3ga
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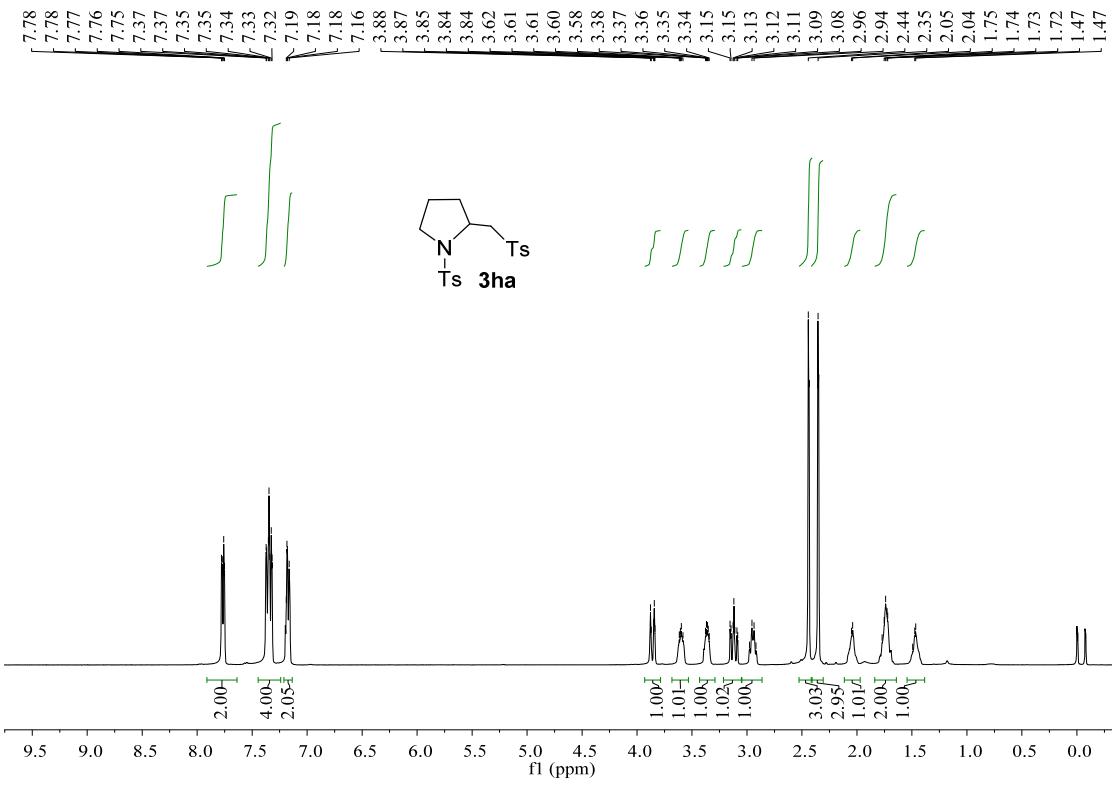
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.34
7.33
7.32
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7.18
7.16
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3.87
3.85
3.84
3.84
3.62
3.61
3.61
3.60
3.58
3.38
3.37
3.36
3.35
3.34
3.15
3.15
3.13
3.12
3.11
3.09
3.08
2.96
2.94
2.44
2.35
2.05
2.04
1.75
1.74
1.73
1.72
1.47
1.47
Ts
N
Ts
3ha
2.00
4.00
2.05
1.00
1.01
1.00
1.02
1.00
3.03
2.95
1.01
2.00
1.00
9.5
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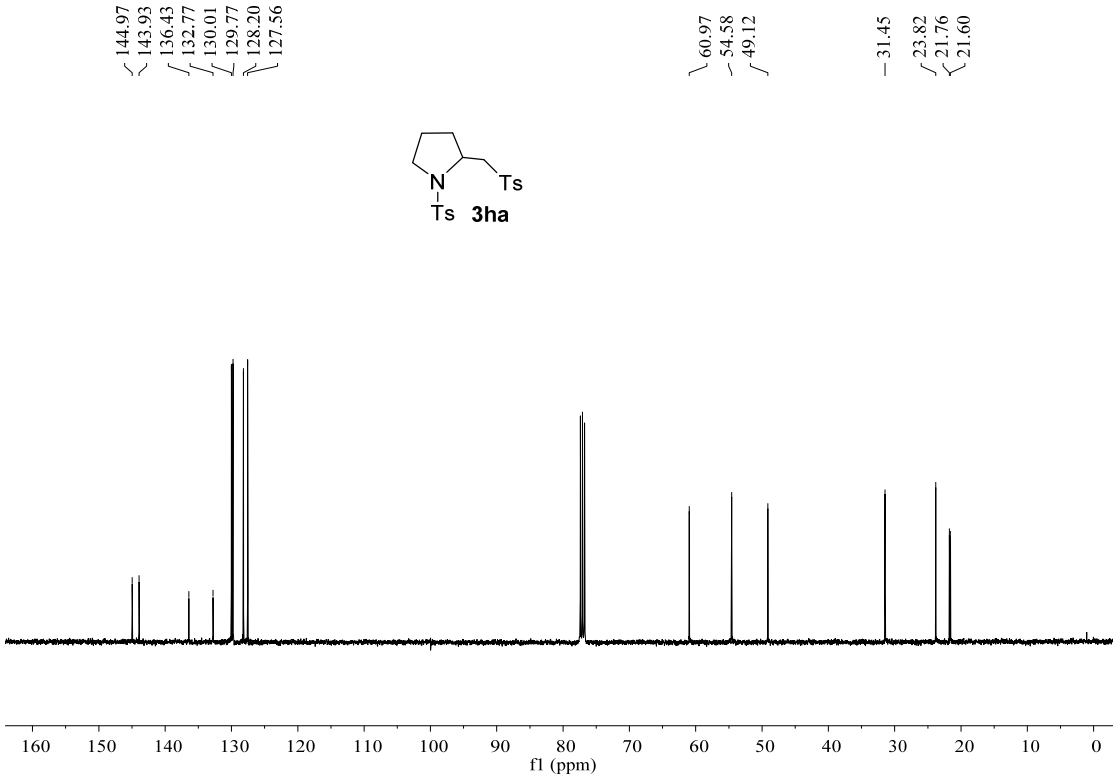
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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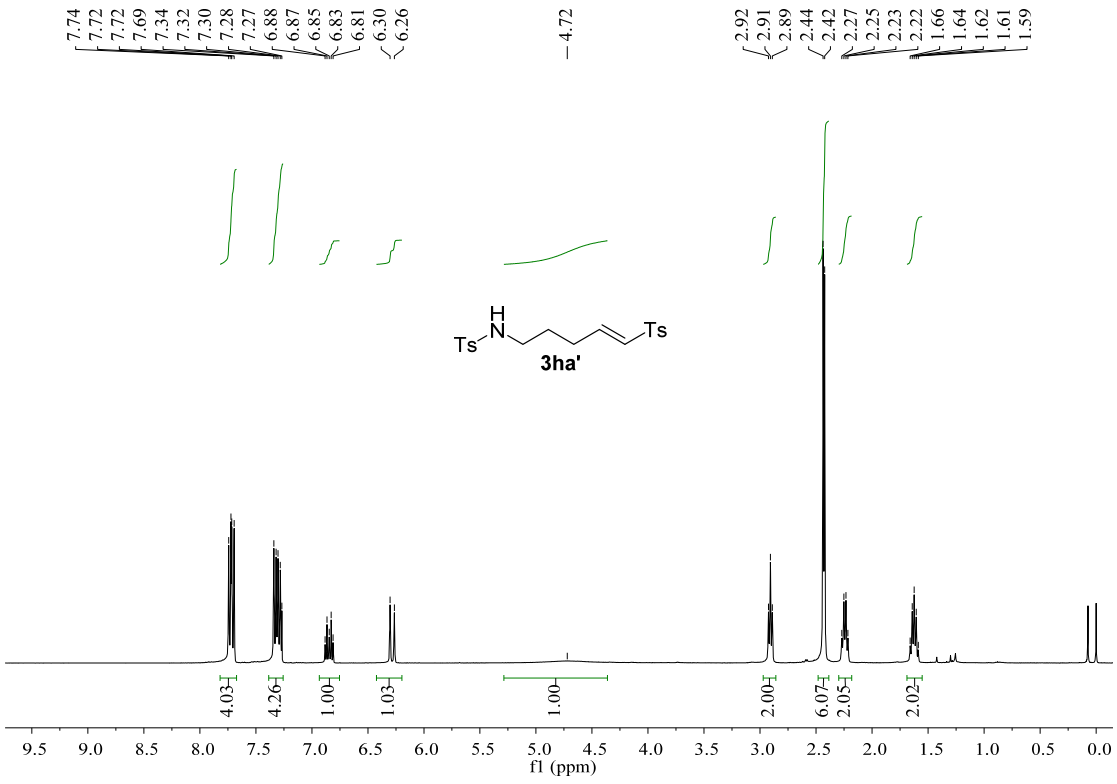
54.58
49.12
31.45
23.82
21.76
21.60
Ts
N
Ts
3ha
f1 (ppm)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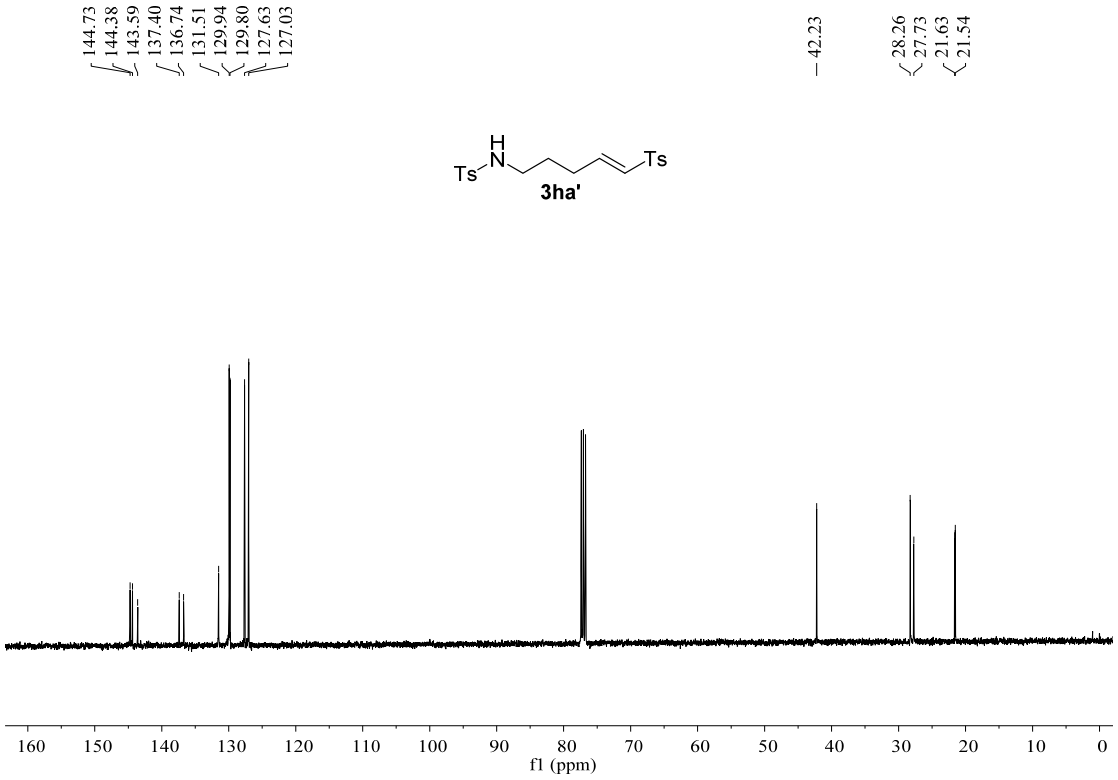
7.27
6.88
6.87
6.85
6.83
6.81
6.30
6.26
4.72
2.92
2.91
2.89
2.44
2.42
2.27
2.25
2.23
2.22
1.66
1.64
1.62
1.61
1.59
H
N
Ts
Ts
3ha'
4.03
4.26
1.00
1.03
1.00
2.00
6.07
2.05
2.02
f1 (ppm)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127.03
42.23
28.26
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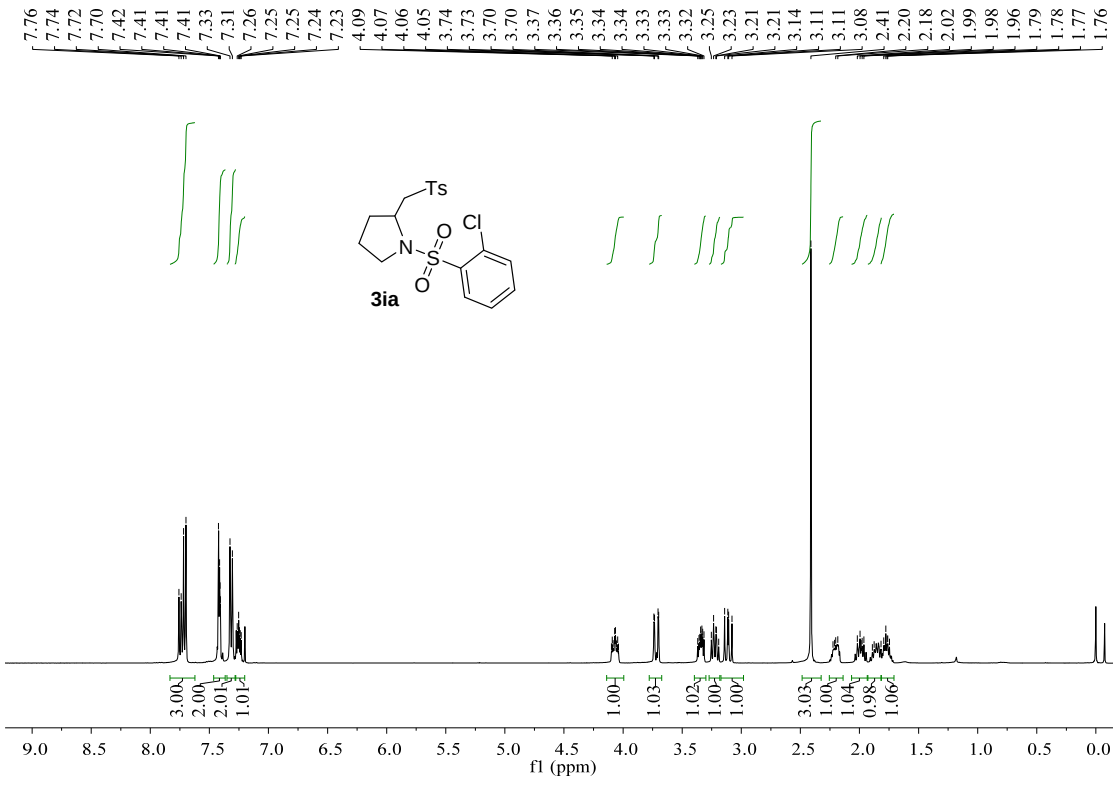
21.63
21.54
Ts
H
N
Ts
3ha'
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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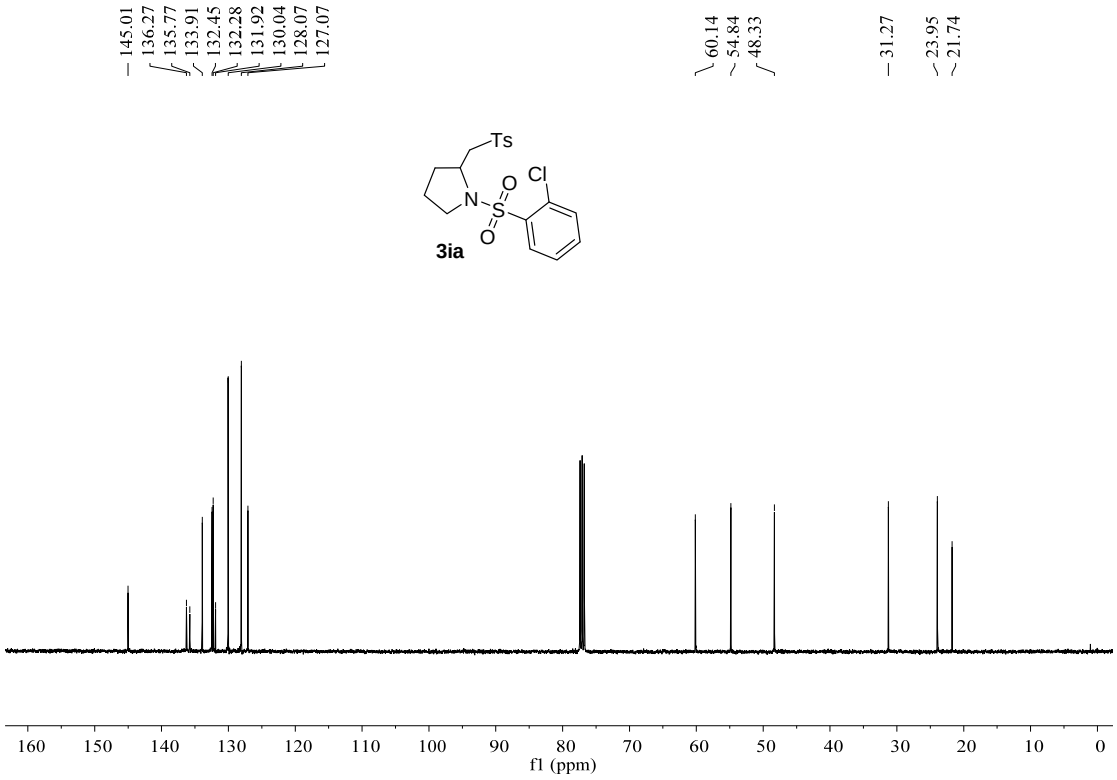
4.09 4.07 4.06 4.05 3.74 3.73 3.70 3.70 3.37 3.36 3.35 3.34 3.34 3.33 3.33 3.32 3.25 3.23 3.21 3.21 3.14 3.11 3.11 3.08 2.41 2.20 2.18 2.02 1.99 1.98 1.96 1.79 1.78 1.77 1.76
Ts
Cl
N
S
O
O
3ia
3.00 2.00 2.01 1.01
1.00 1.03 1.02 1.00 1.00
3.03 1.00 1.04 0.98 1.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.04
128.07
127.07
60.14
54.84
48.33
31.27
23.95
21.74
Ts
Cl
N
S
O
O
3ia
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90
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70
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50
40
30
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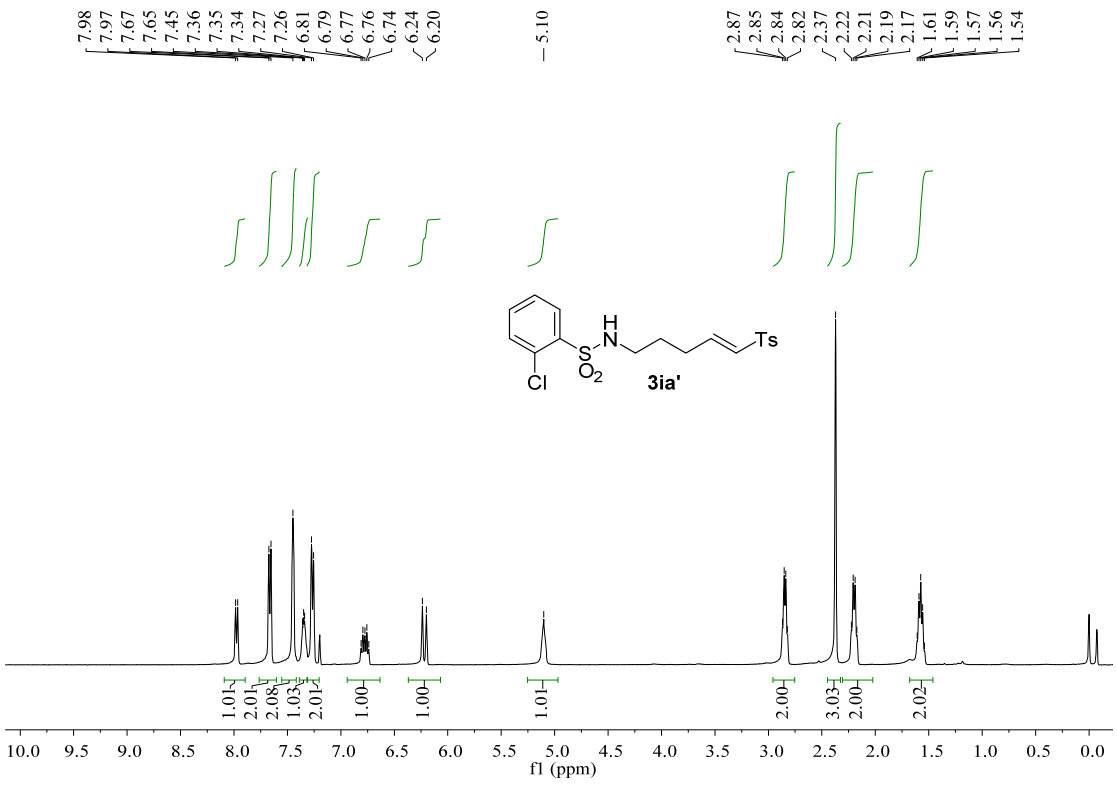
0
f1 (ppm)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6.74
6.24
6.20
5.10
2.87
2.85
2.84
2.82
2.37
2.22
2.21
2.19
2.17
1.61
1.59
1.57
1.56
1.54
H
N
Ts
S
O2
Cl
3ia'
1.01
2.01
2.08
1.03
2.01
1.00
1.00
1.01
2.00
3.03
2.00
2.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
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2.0
1.5
1.0
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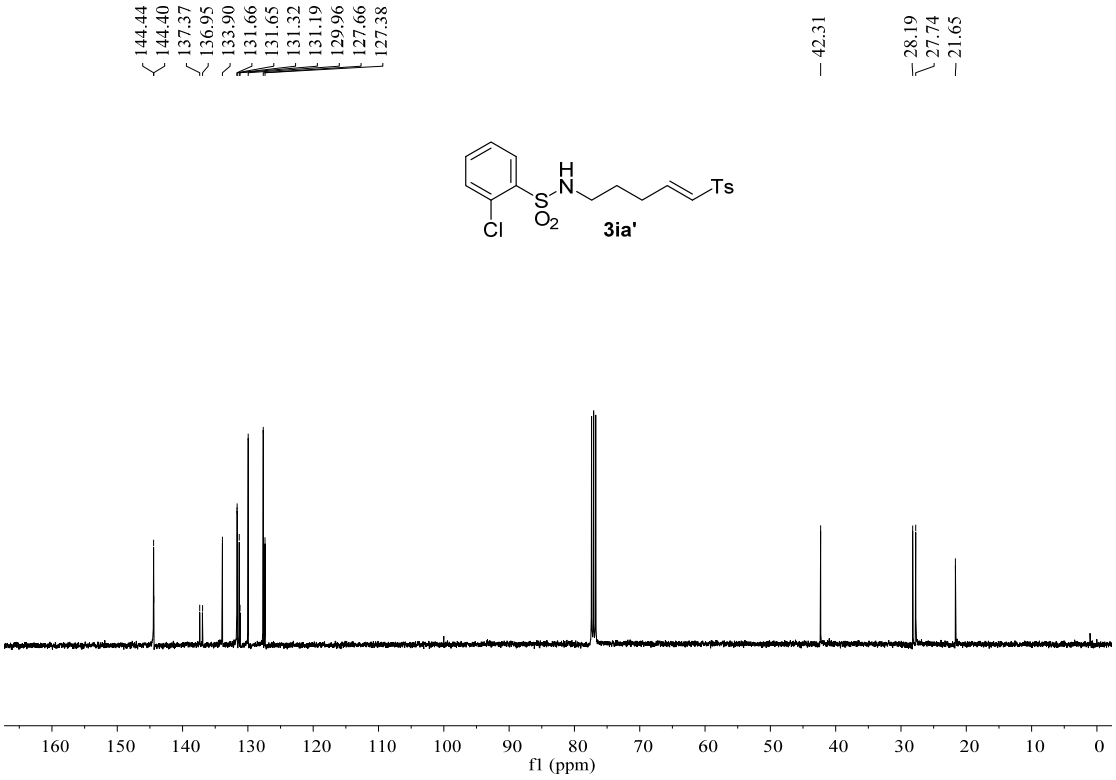
0.0
f1 (ppm)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127.66
127.38
42.31
28.19
27.74
21.65
Cl
S
O2
H
N
Ts
3ia'
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150
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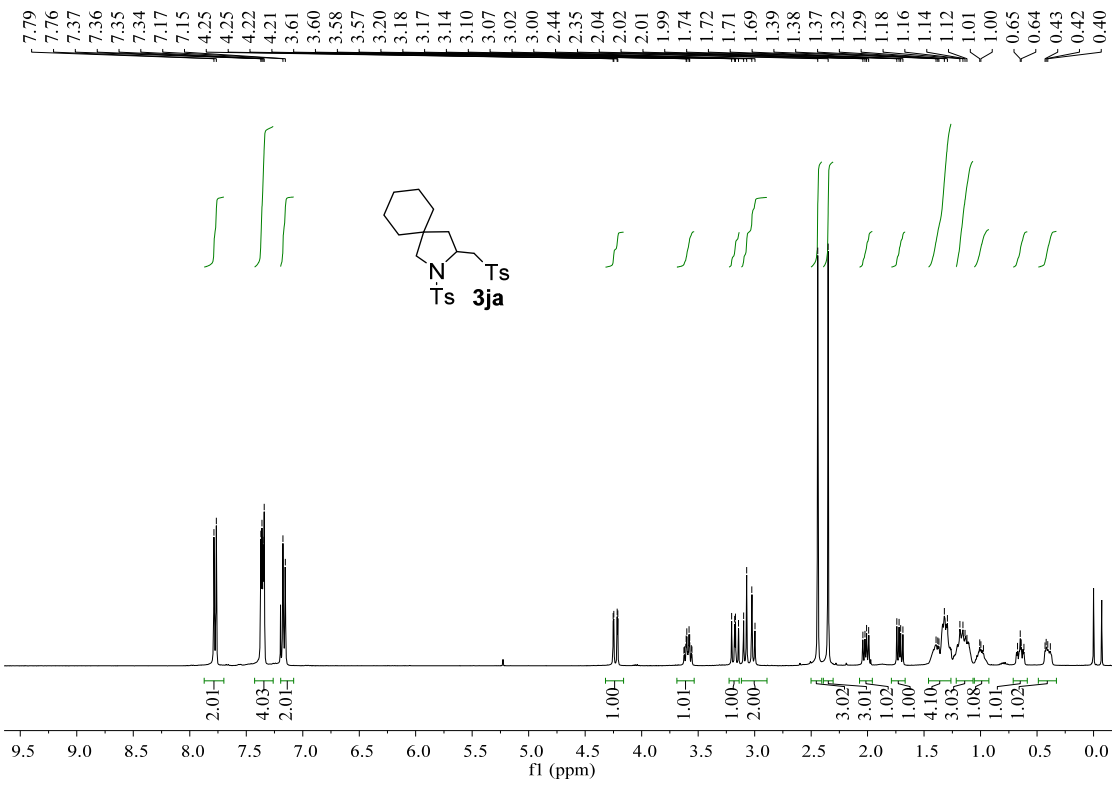
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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3.60
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3.20
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3.17
3.14
3.10
3.07
3.02
3.00
2.44
2.35
2.04
2.02
2.01
1.99
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1.37
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1.29
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1.16
1.14
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0.42
0.40
N
Ts
Ts
3ja
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1.01
1.00
2.00
3.02
3.01
1.02
1.00
4.10
3.03
1.08
1.01
1.02
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7.5
7.0
6.5
6.0
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2.0
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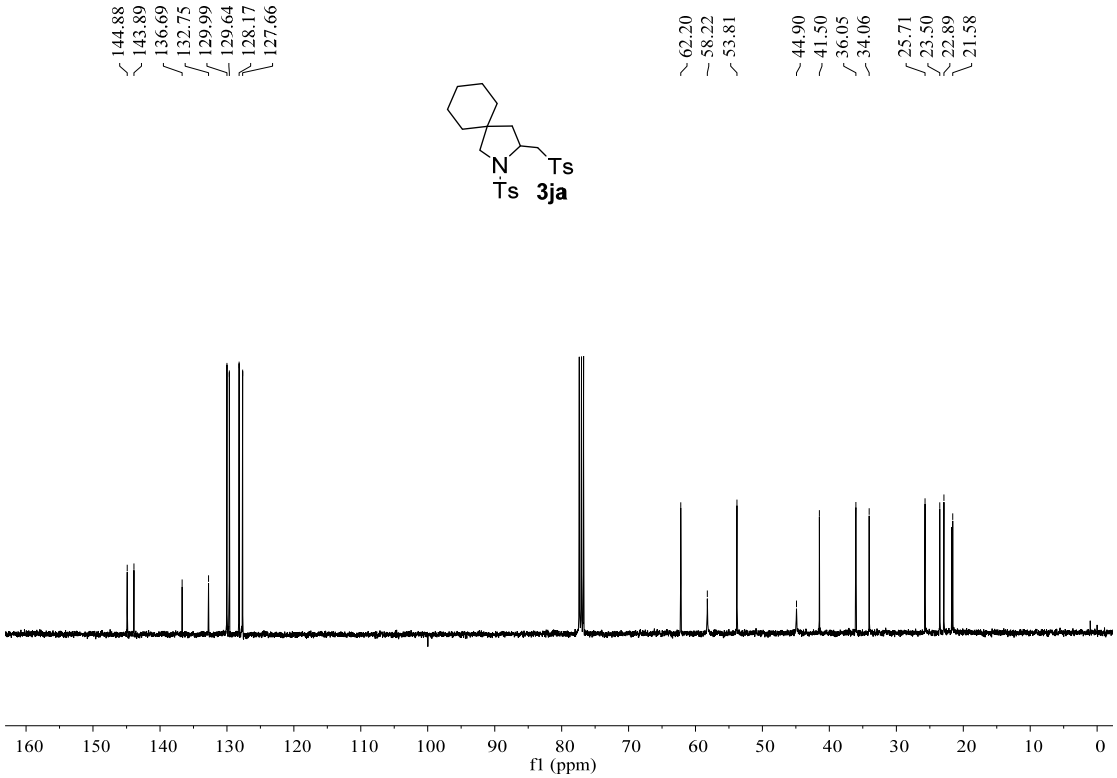
f1 (ppm)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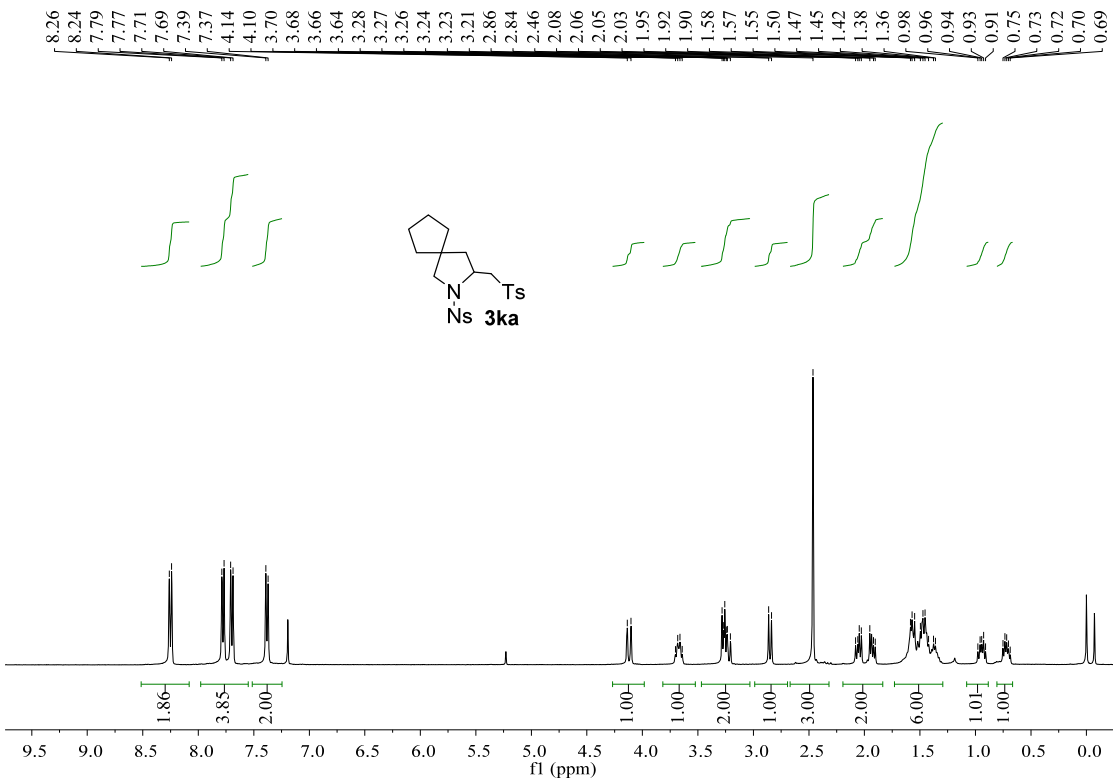
34.06
25.71
23.50
22.89
21.58
N
Ts
Ts
3ja
f1 (ppm)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3.64
3.28
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3.23
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2.46
2.08
2.06
2.05
2.03
1.95
1.92
1.90
1.58
1.57
1.55
1.50
1.47
1.45
1.42
1.38
1.36
0.98
0.96
0.94
0.93
0.91
0.75
0.73
0.72
0.70
0.69
N
Ts
Ns
3ka
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1.00
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1.00
3.00
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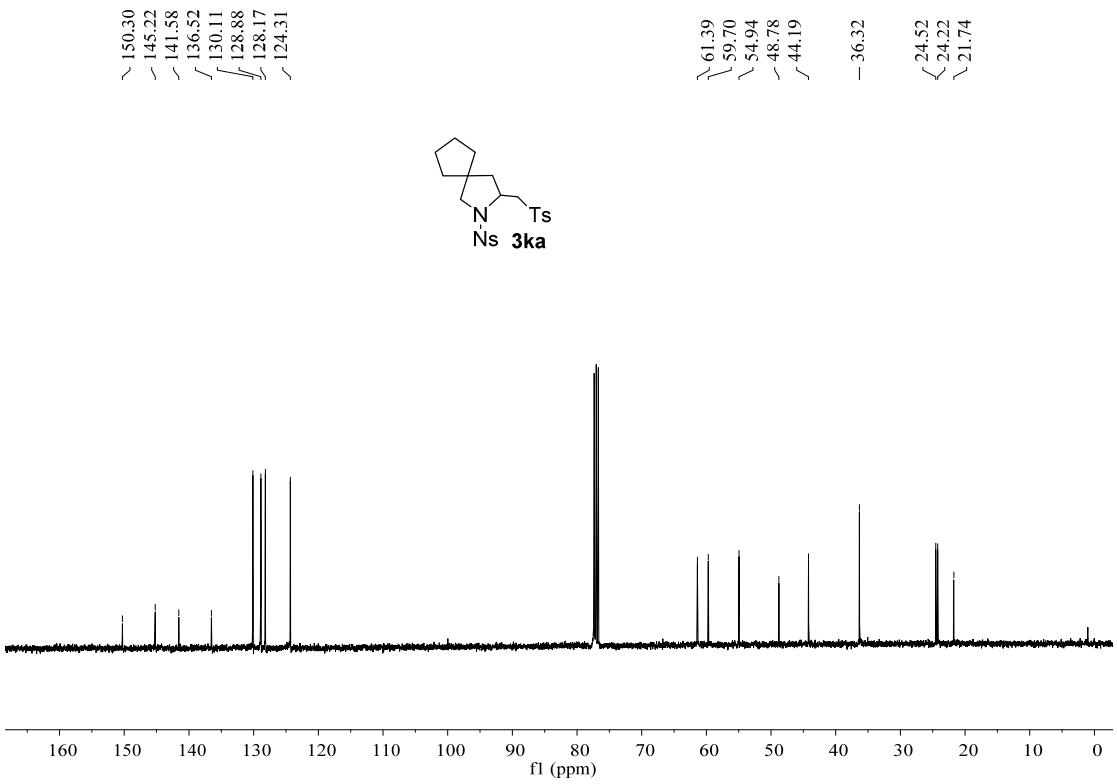
6.00
1.01
1.00
f1 (ppm)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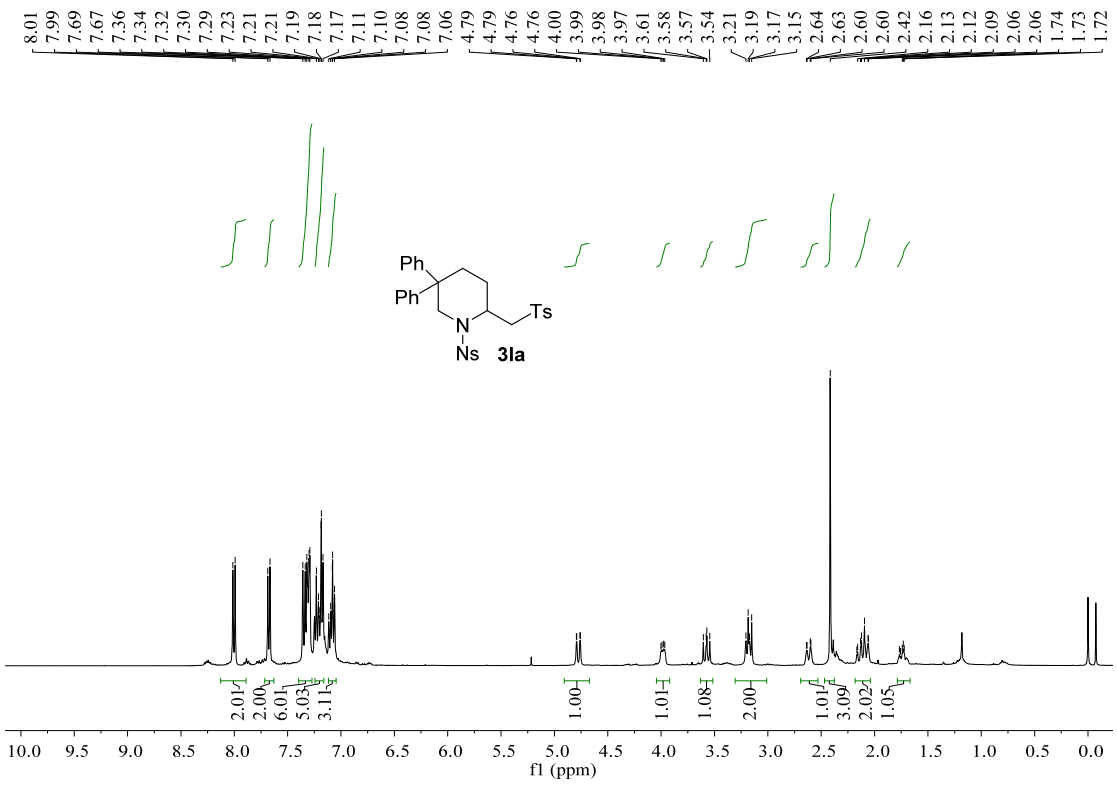
128.17
124.31
61.39
59.70
54.94
48.78
44.19
36.32
24.52
24.22
21.74
Ts
N
Ns
3ka
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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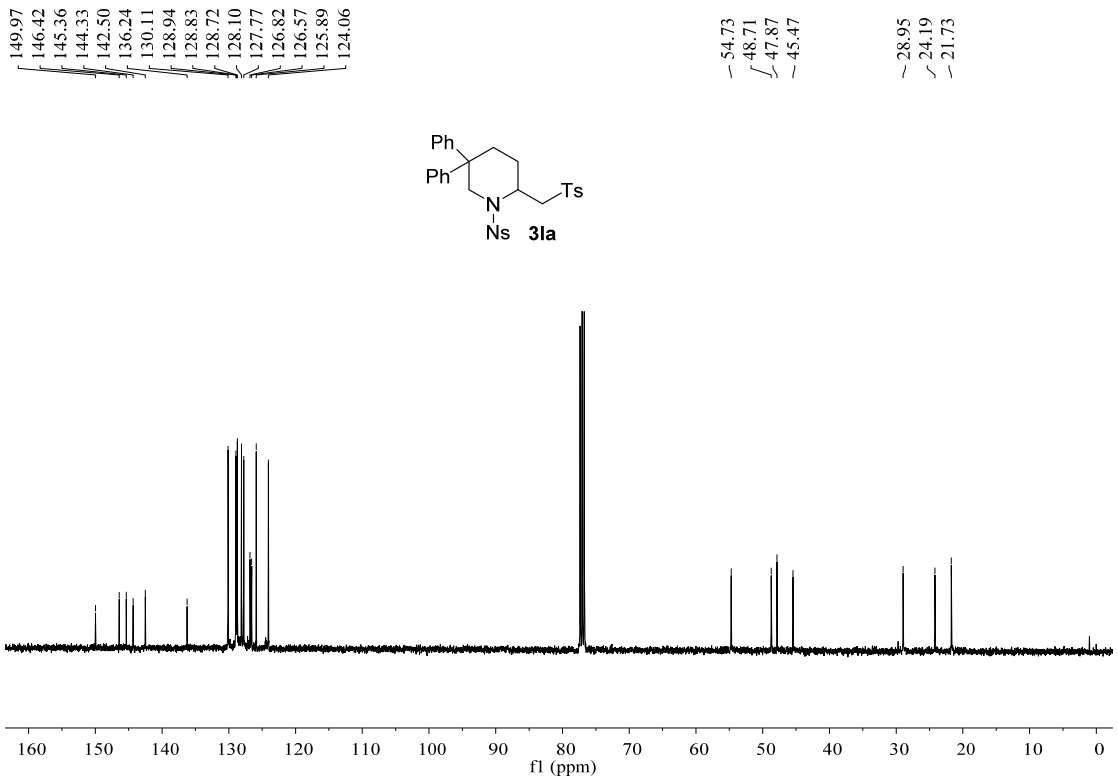
4.79 4.79 4.76 4.76 4.00 3.99 3.98 3.97 3.61 3.58 3.57 3.54
3.21 3.19 3.17 3.15
2.64 2.63 2.60 2.60 2.42 2.16 2.13 2.12 2.09 2.06 2.06 1.74 1.73 1.72
Ph
Ph
Ts
N
Ns
3la
2.01 2.00 6.01 5.03 3.11 1.00 1.01 1.08 2.00 1.01 3.09 2.02 1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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145.36
144.33
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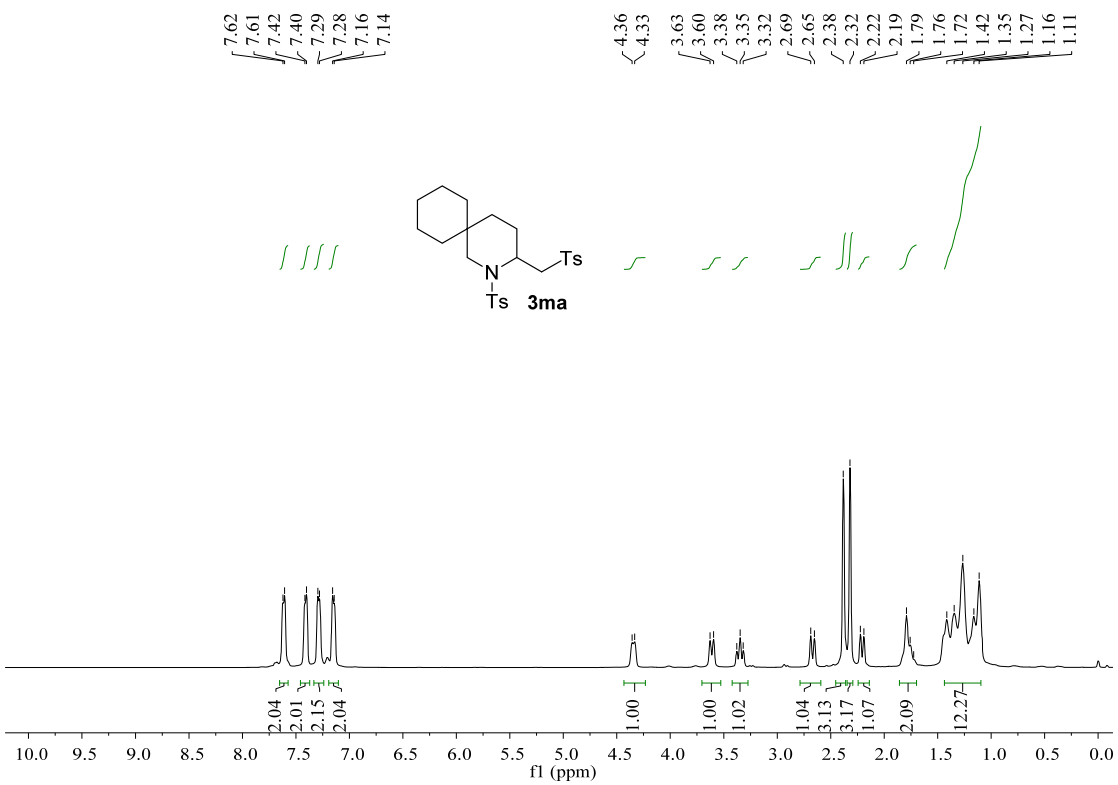
128.94
128.83
128.72
128.10
127.77
126.82
126.57
125.89
124.06
54.73
48.71
47.87
45.47
28.95
24.19
21.73
Ph
Ph
Ts
N
Ns
3la
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.16
7.14
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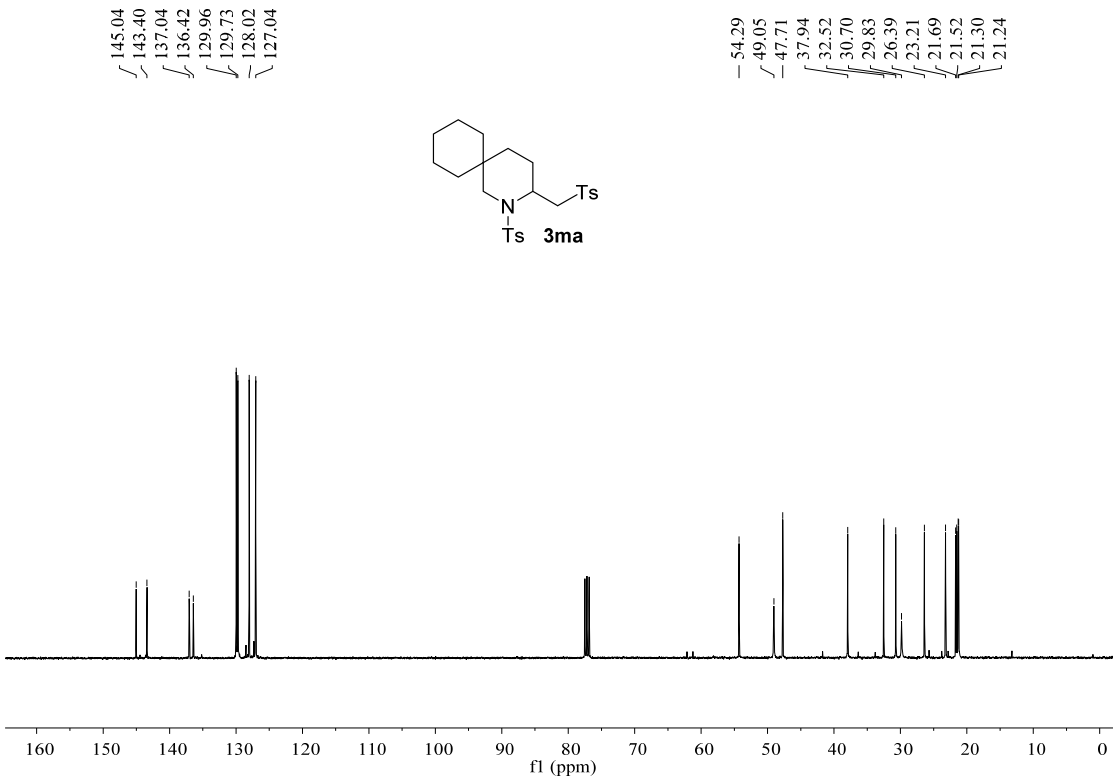
4.33
3.63
3.60
3.38
3.35
3.32
2.69
2.65
2.38
2.32
2.22
2.19
1.79
1.76
1.72
1.42
1.35
1.27
1.16
1.11
Ts
N
Ts
3ma
2.04
2.01
2.15
2.04
1.00
1.00
1.02
1.04
3.13
3.17
1.07
2.09
12.27
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.04
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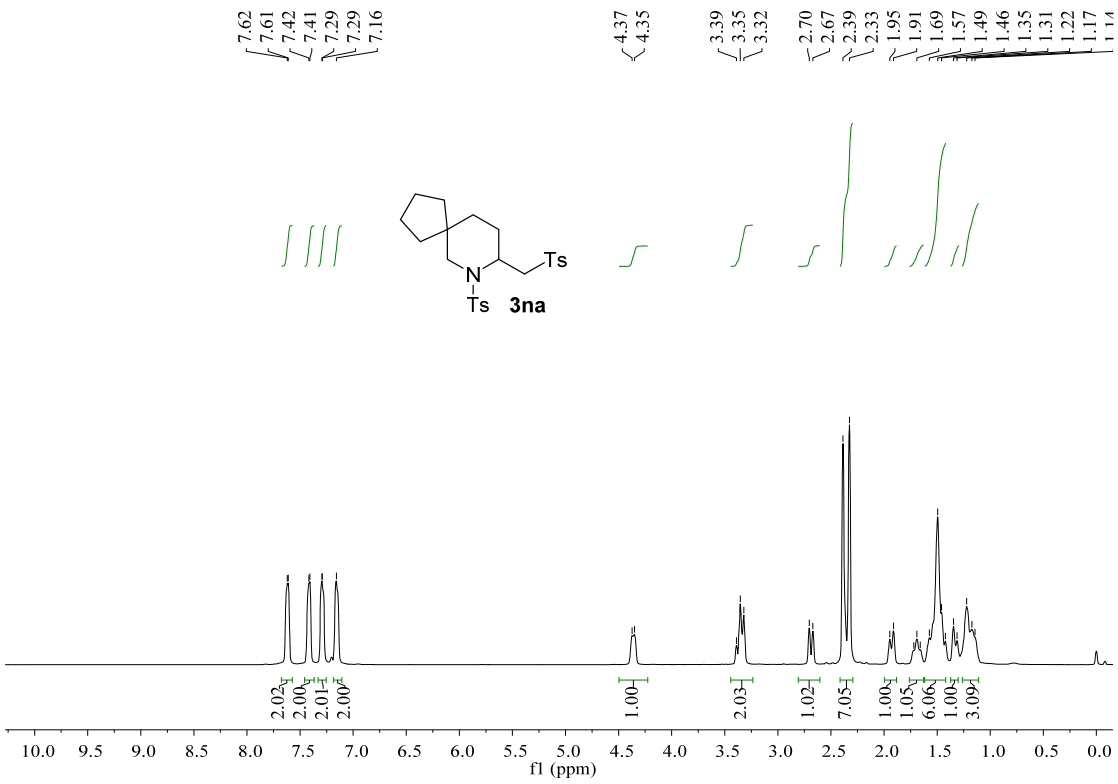
129.73
128.02
127.04
54.29
49.05
47.71
37.94
32.52
30.70
29.83
26.39
23.21
21.69
21.52
21.30
21.24
Ts
N
Ts
3ma
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.61
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7.16
4.37
4.35
3.39
3.35
3.32
2.70
2.67
2.39
2.33
1.95
1.91
1.69
1.57
1.49
1.46
1.35
1.31
1.22
1.17
Ts
N
Ts
3na
2.02
2.00
2.01
2.00
1.00
2.03
1.02
7.05
1.00
1.05
6.06
1.00
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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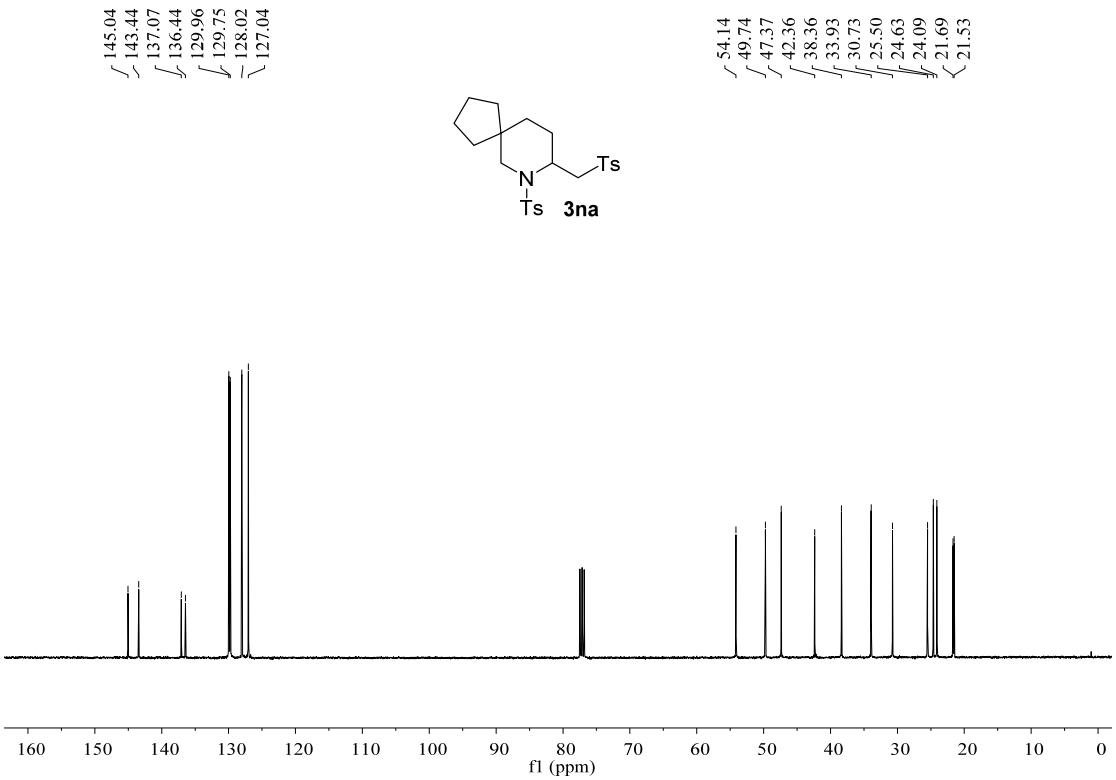
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129.75
128.02
127.04
54.14
49.74
47.37
42.36
38.36
33.93
30.73
25.50
24.63
24.09
21.69
21.53
Ts
N
Ts
3na
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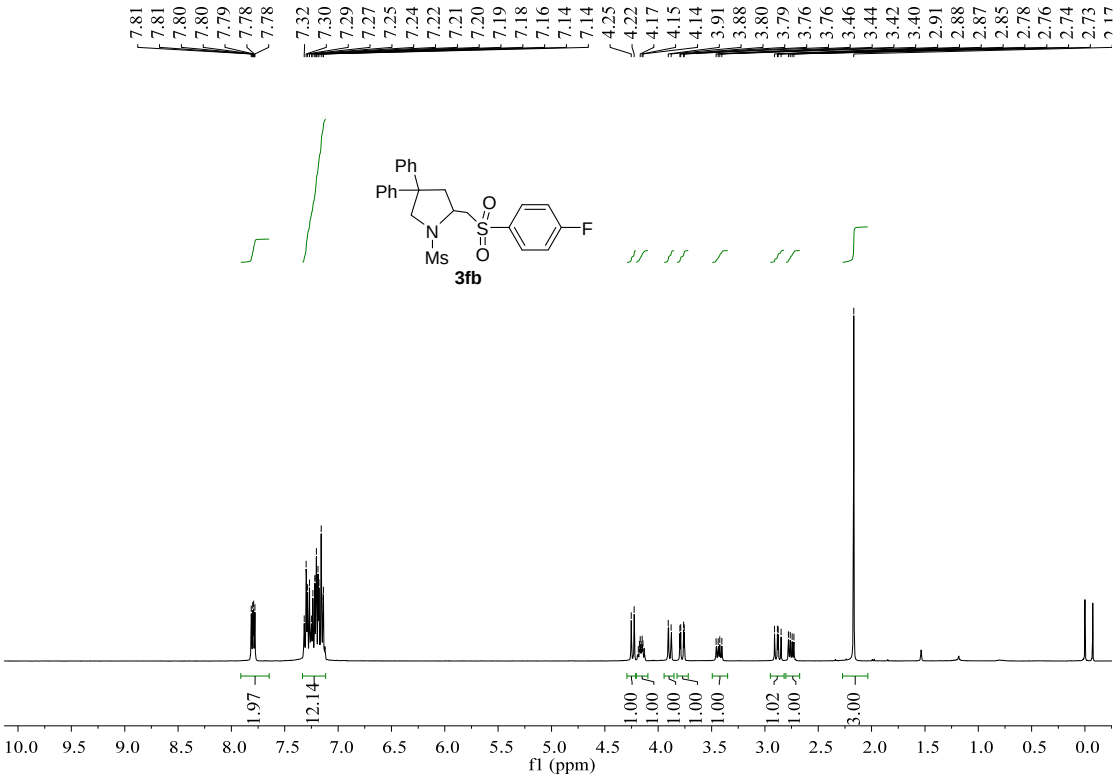
f1 (ppm)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7.80
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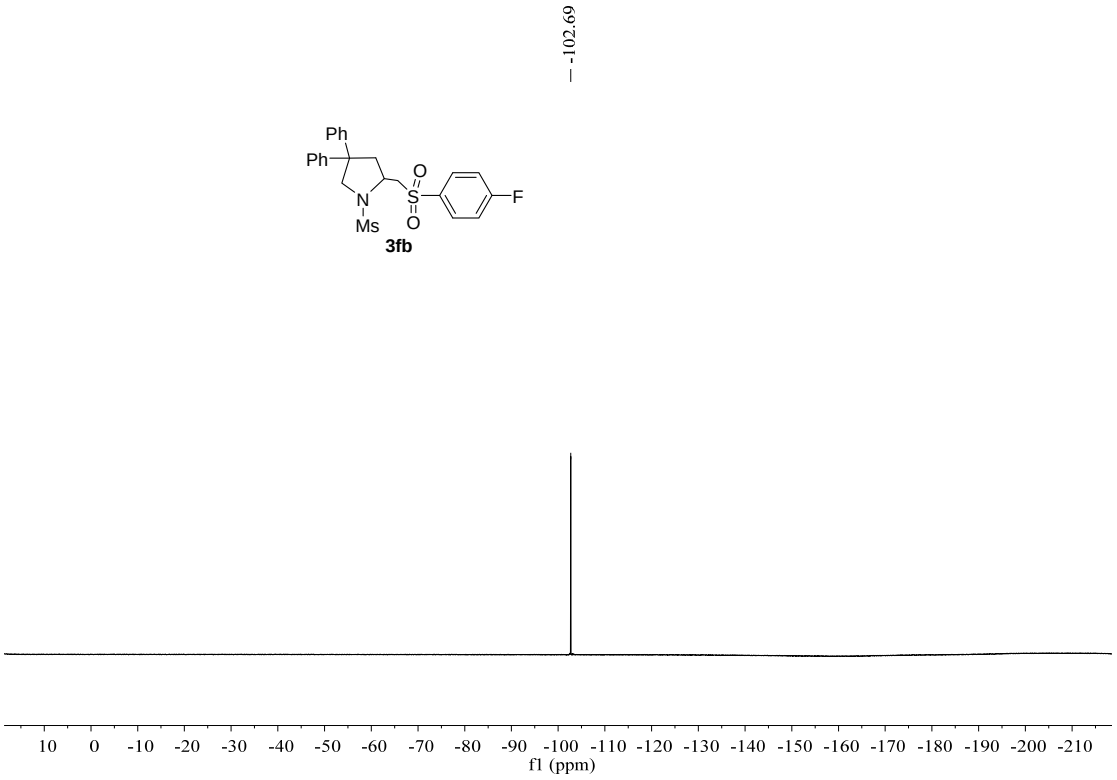
7.78
7.78
7.32
7.30
7.29
7.27
7.25
7.24
7.22
7.21
7.20
7.19
7.18
7.16
7.14
7.14
4.25
4.22
4.17
4.15
4.14
3.91
3.88
3.80
3.79
3.76
3.76
3.46
3.44
3.42
3.40
2.91
2.88
2.87
2.85
2.78
2.76
2.74
2.73
Ph
Ph
N
Ms
O
S
O
F
3fb
1.97
12.14
1.00
1.00
1.00
1.00
1.00
1.02
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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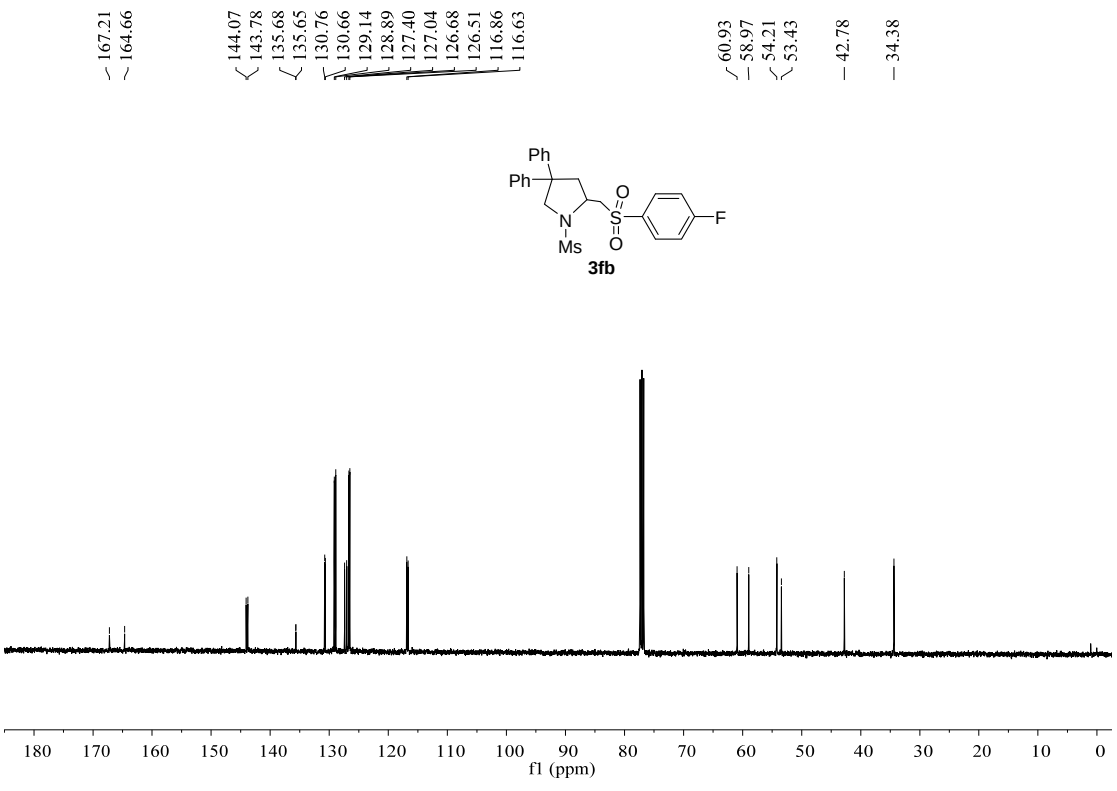
Ph
Ph
N
Ms
O
S
O
F
3fb
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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164.66
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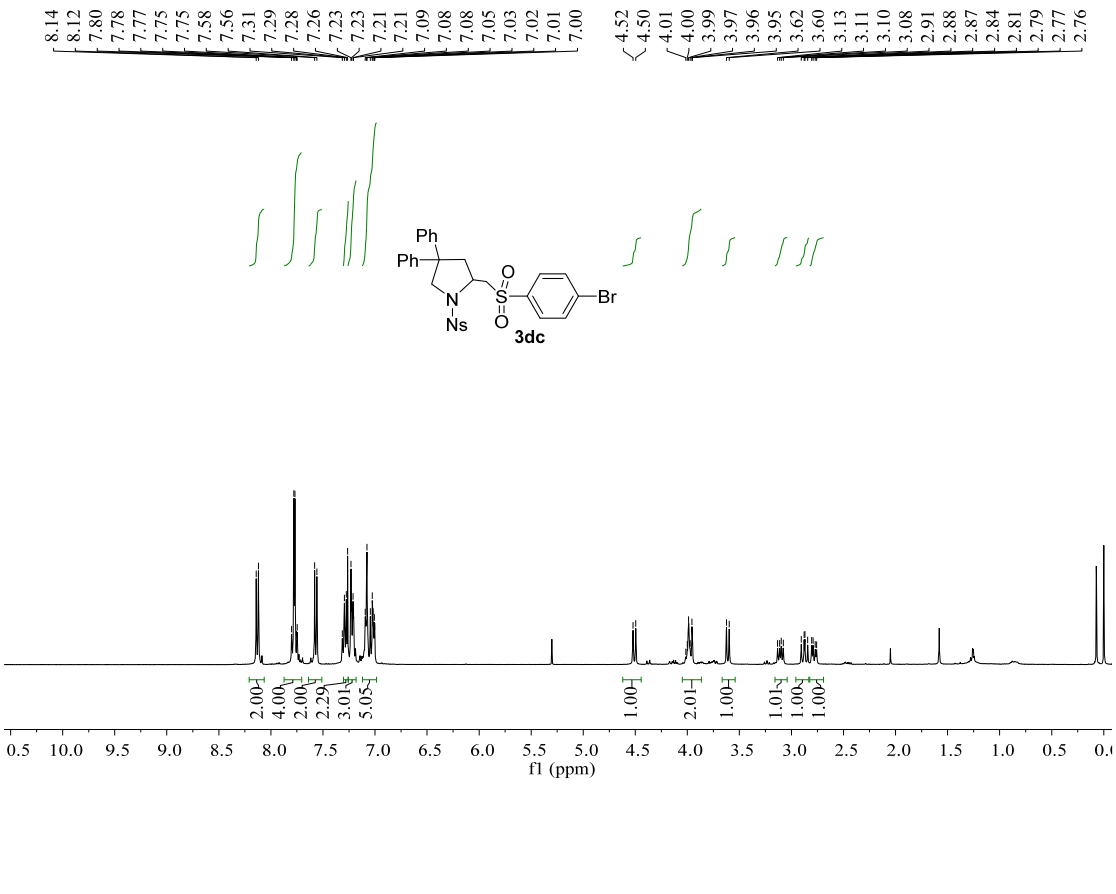
135.68
135.65
130.76
130.66
129.14
128.89
127.40
127.04
126.68
126.51
116.86
116.63
60.93
58.97
54.21
53.43
42.78
34.38
Ph
Ph
N
Ms
O
S
O
F
3fb
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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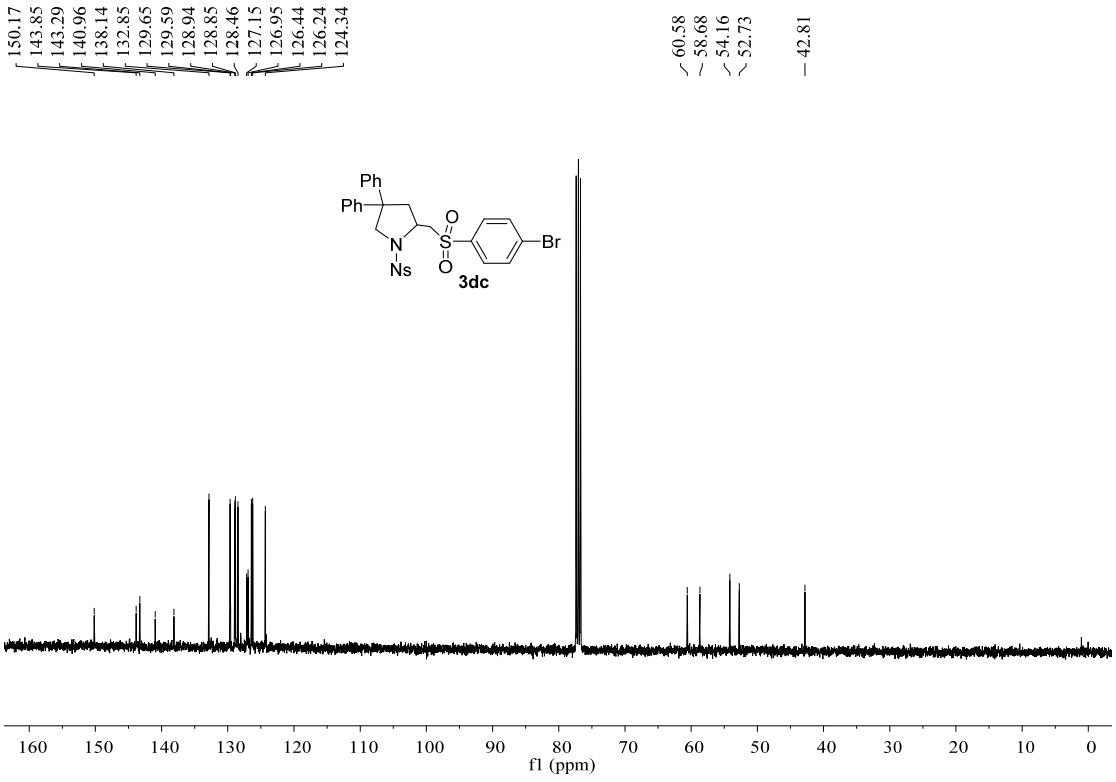
7.75
7.75
7.58
7.56
7.31
7.29
7.28
7.26
7.23
7.23
7.21
7.21
7.09
7.08
7.08
7.05
7.03
7.02
7.01
7.00
4.52
4.50
4.01
4.00
3.99
3.97
3.96
3.95
3.62
3.60
3.13
3.11
3.10
3.08
2.91
2.88
2.87
2.84
2.81
2.79
2.77
2.76
Ph
Ph
N
Ns
O
S
O
O
Br
3dc
2.00
4.00
2.00
2.29
3.01
5.05
1.00
2.01
1.00
1.01
1.00
1.00
f1 (ppm)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143.29
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138.14
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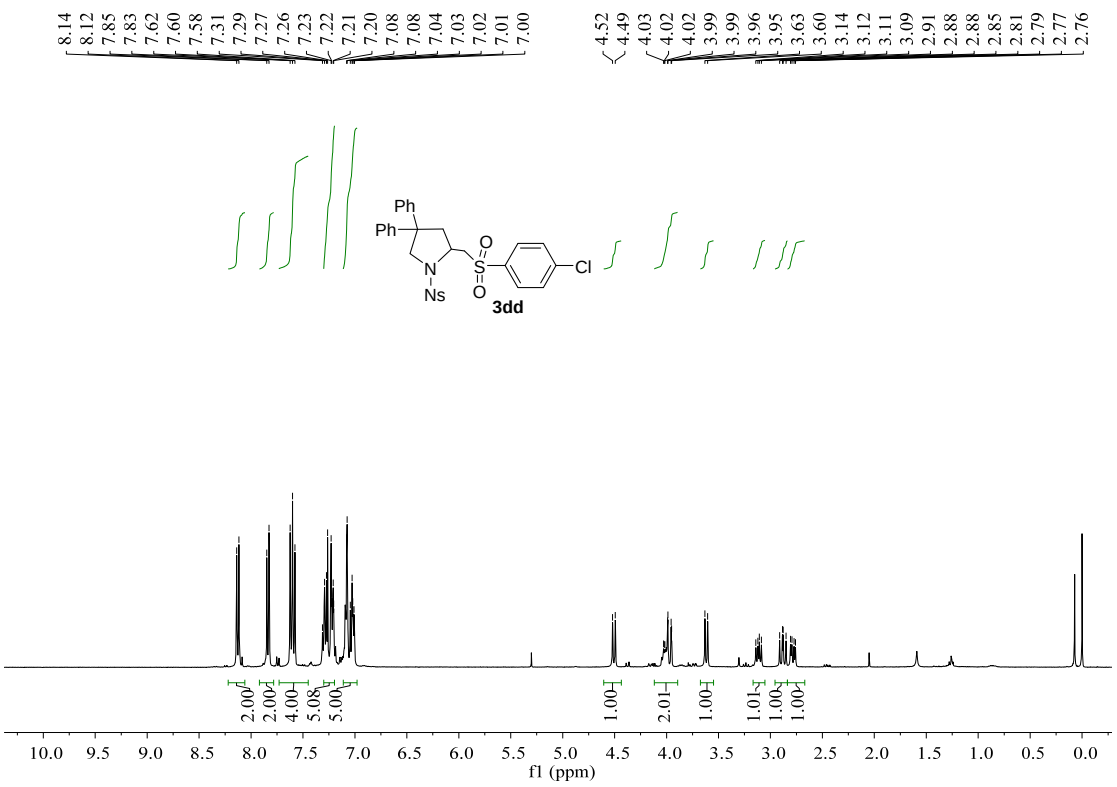
129.59
128.94
128.85
128.46
127.15
126.95
126.44
126.24
124.34
60.58
58.68
54.16
52.73
42.81
Ph
Ph
N
Ns
O
S
O
O
Br
3dc
f1 (ppm)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8.12
7.85
7.83
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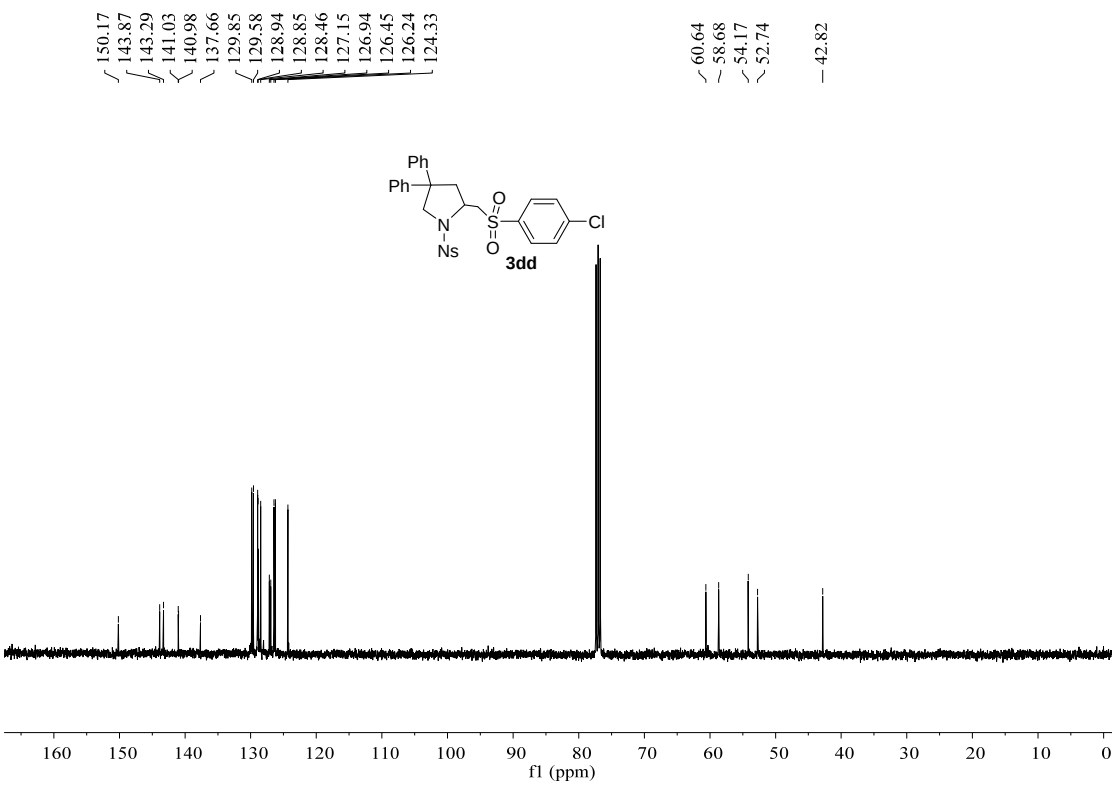
7.60
7.58
7.31
7.29
7.27
7.26
7.23
7.22
7.21
7.20
7.08
7.08
7.04
7.03
7.02
7.01
7.00
4.52
4.49
4.03
4.02
4.02
3.99
3.99
3.96
3.95
3.63
3.60
3.14
3.12
3.11
3.09
2.91
2.88
2.88
2.85
2.81
2.79
2.77
2.76
Ph
Ph
N
Ns
O
S
O
O
Cl
3dd
2.00
2.00
4.00
5.08
5.00
1.00
2.01
1.00
1.01
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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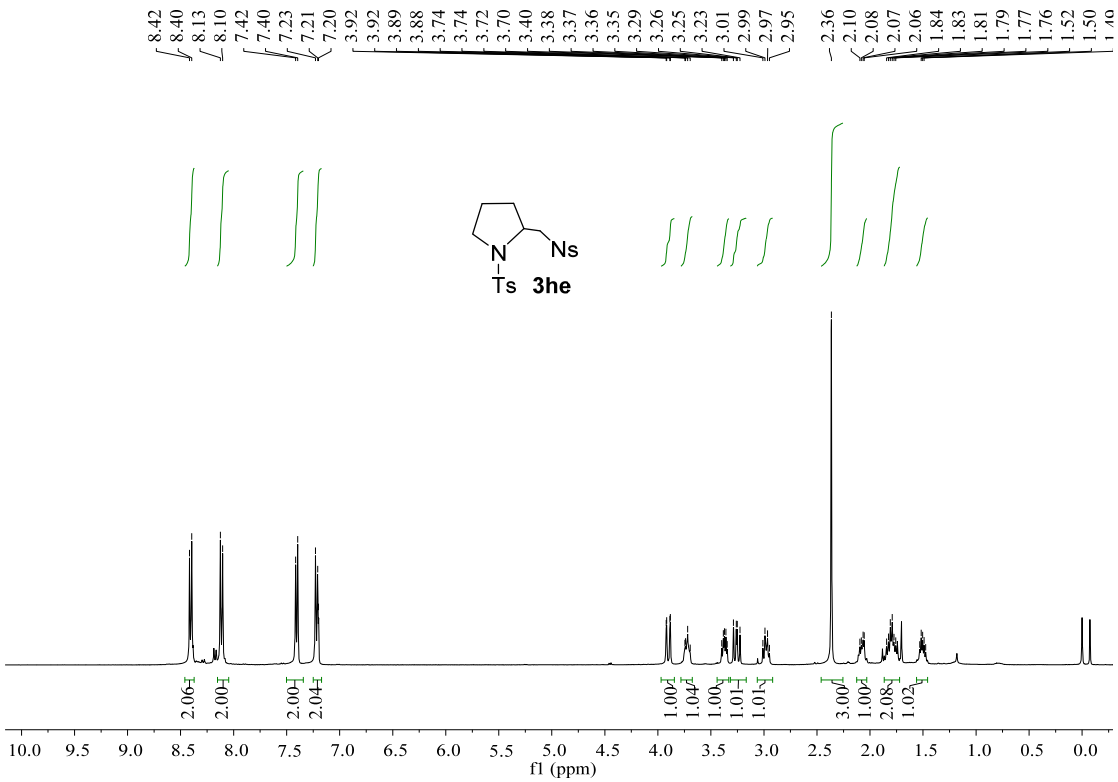
137.66
129.85
129.58
128.94
128.85
128.46
127.15
126.94
126.45
126.24
124.33
60.64
58.68
54.17
52.74
42.82
Ph
Ph
N
Ns
O
S
O
O
Cl
3dd
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.40
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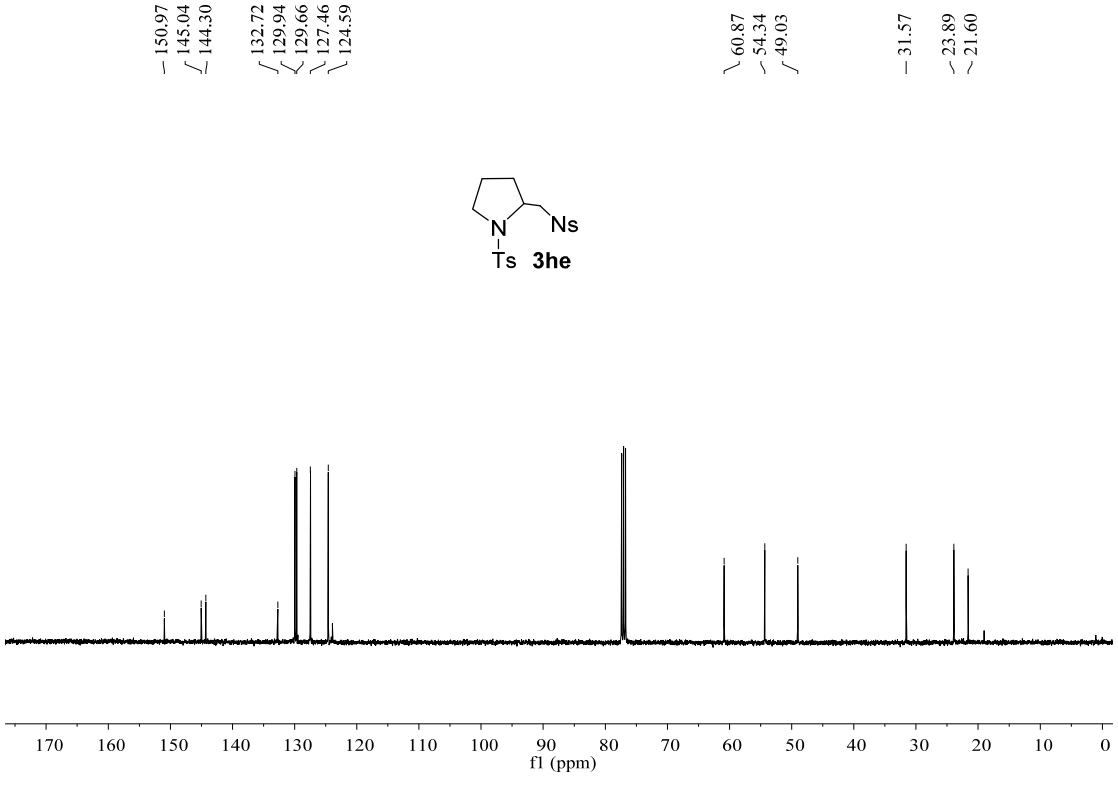
3.88
3.74
3.74
3.72
3.70
3.40
3.38
3.37
3.36
3.35
3.29
3.26
3.25
3.23
3.01
2.99
2.97
2.95
2.36
2.10
2.08
2.07
2.06
1.84
1.83
1.81
1.79
1.77
1.76
1.52
1.50
Ns
Ts
3he
2.06
2.00
2.00
2.04
1.00
1.04
1.00
1.01
1.01
3.00
1.00
2.08
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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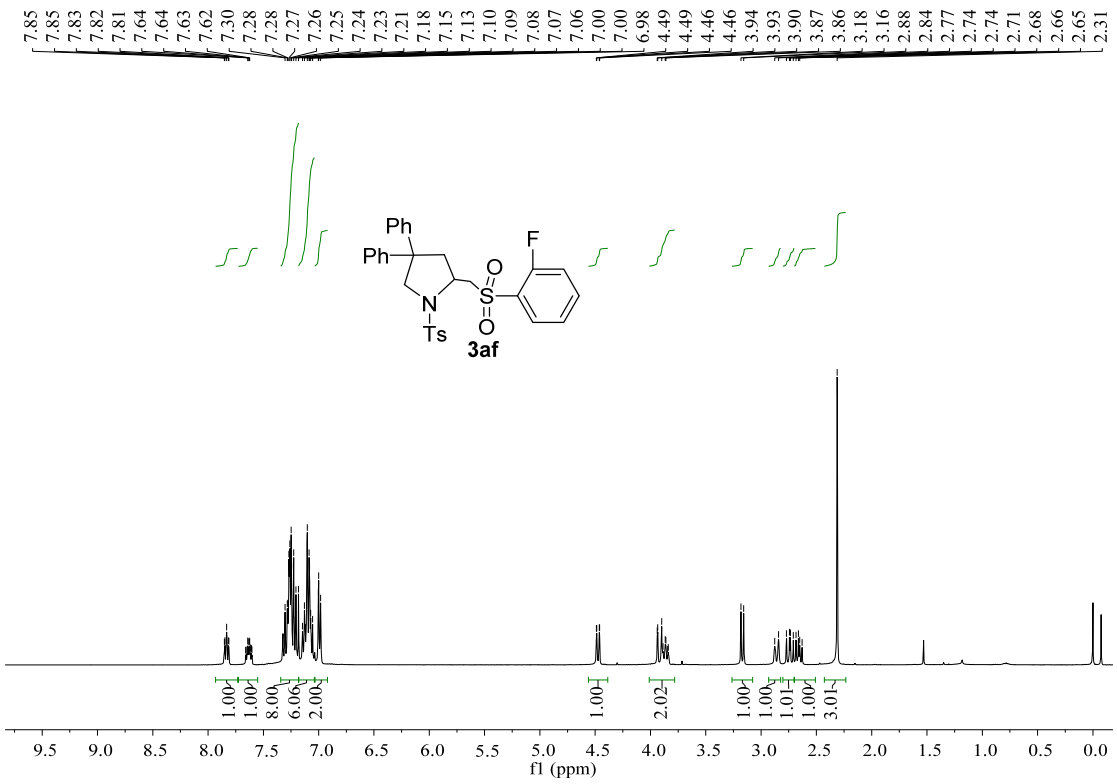
129.94
129.66
127.46
124.59
60.87
54.34
49.03
31.57
23.89
21.60
Ns
Ts
3he
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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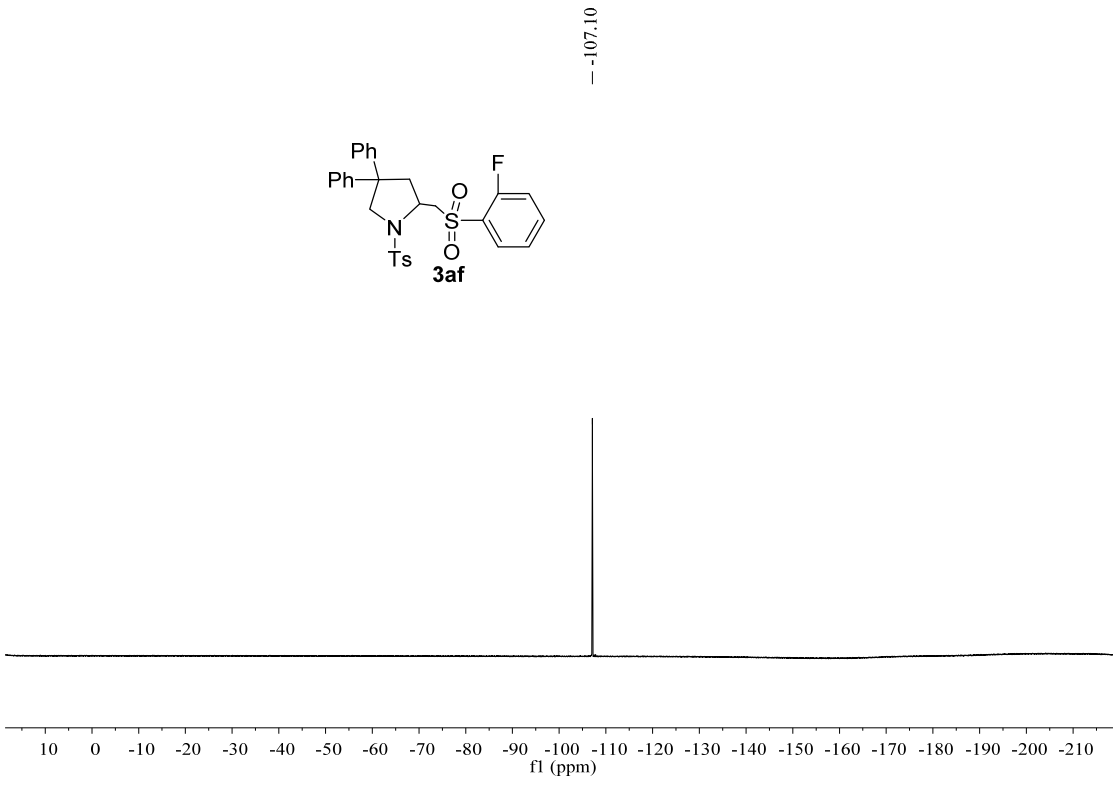
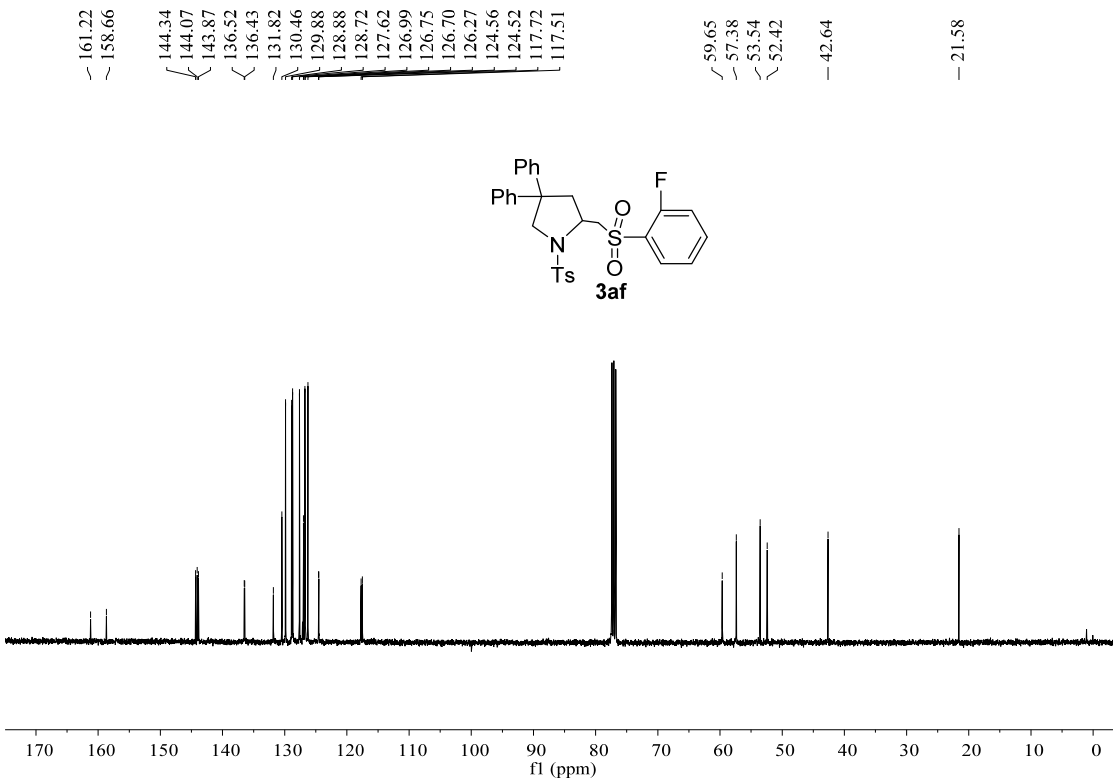
Ph
Ph
F
O
S
O
N
Ts
3af
1.00 1.00 8.00 6.06 2.00 1.00 2.02 1.00 1.00 1.01 1.00 3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-107.10
Ph
Ph
F
O
S
O
N
Ts
3af
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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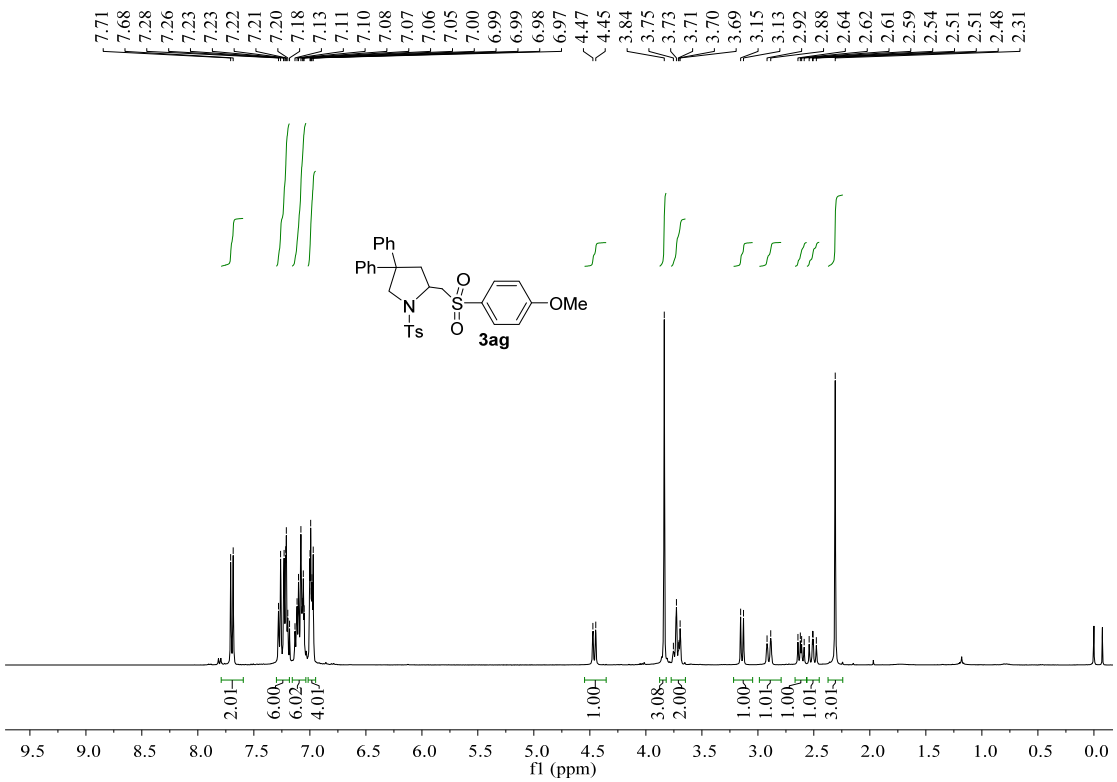
128.88
128.72
127.62
126.99
126.75
126.70
126.27
124.56
124.52
117.72
117.51
59.65
57.38
53.54
52.42
42.64
21.58
Ph
Ph
F
O
S
O
N
Ts
3af
f1 (ppm)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7.18
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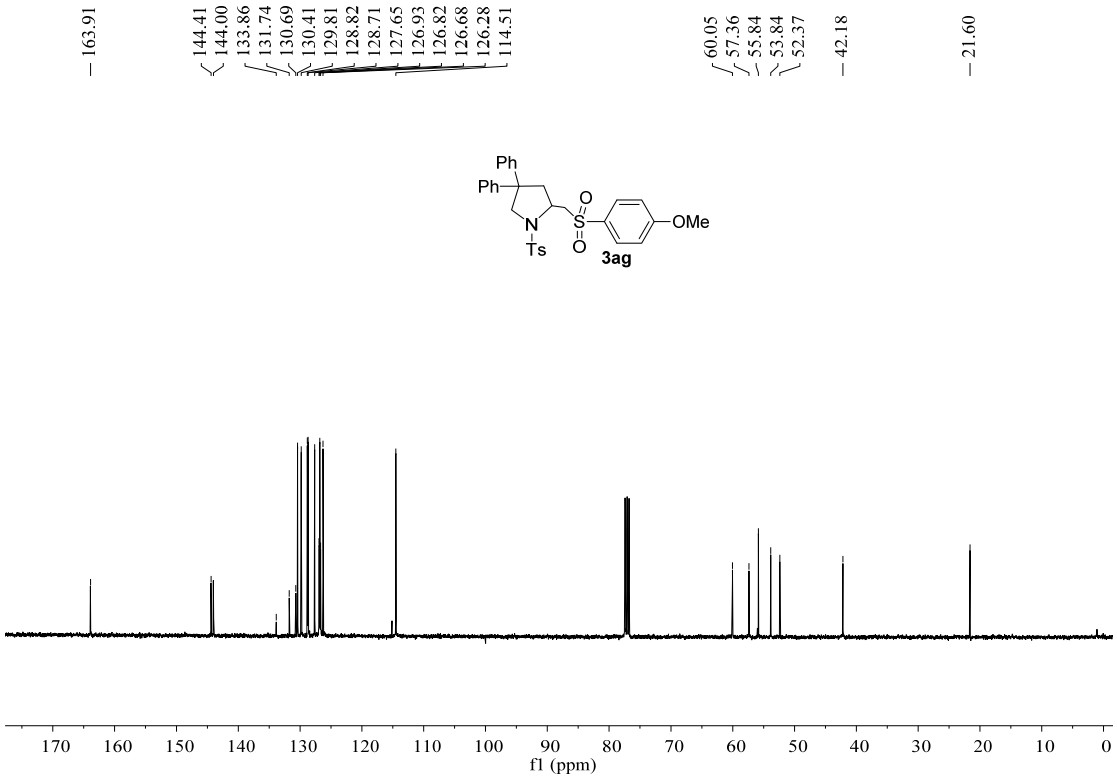
7.11
7.10
7.08
7.07
7.06
7.05
7.00
6.99
6.99
6.98
6.97
4.47
4.45
3.84
3.75
3.73
3.71
3.70
3.69
3.15
3.13
2.92
2.88
2.64
2.62
2.61
2.59
2.54
2.51
2.51
2.48
2.31
Ph
Ph
O
S
O
N
Ts
OMe
3ag
2.01
6.00
6.02
4.01
1.00
3.08
2.00
1.00
1.01
1.00
1.01
3.01
f1 (ppm)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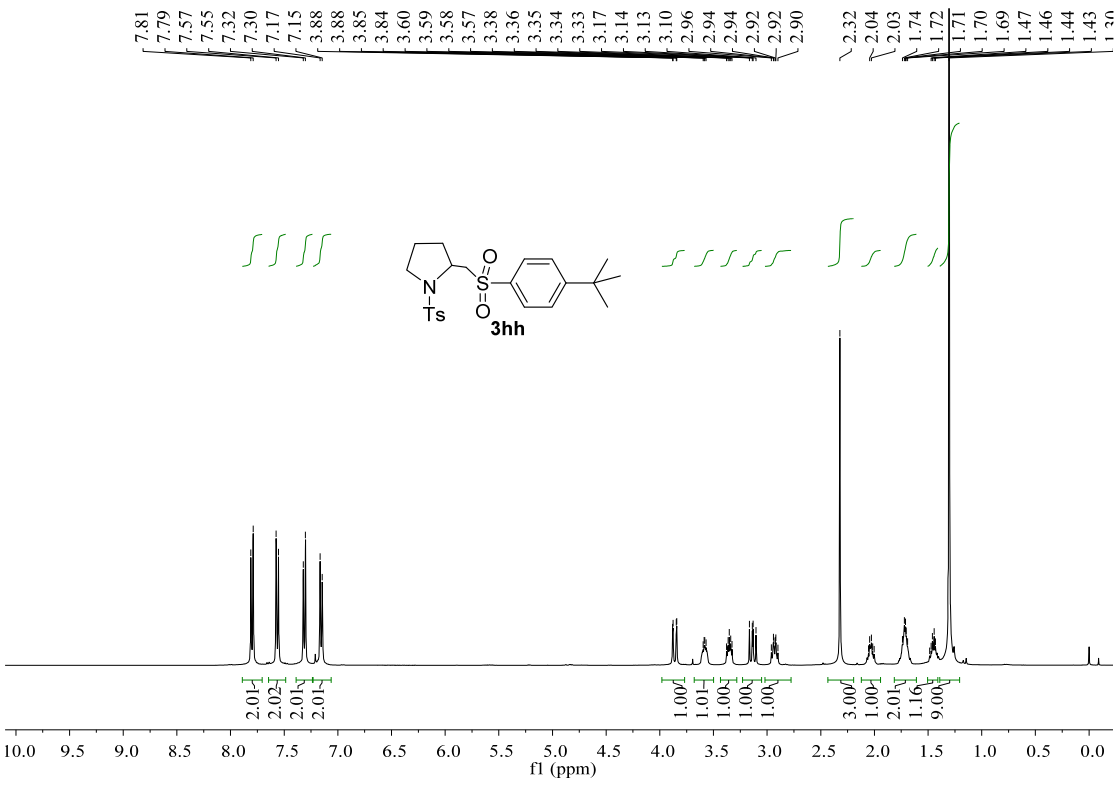
130.41
129.81
128.82
128.71
127.65
126.93
126.82
126.68
126.28
114.51
60.05
57.36
55.84
53.84
52.37
42.18
21.60
Ph
Ph
N
Ts
O
S
O
OMe
3ag
f1 (ppm)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3.88
3.85
3.84
3.60
3.59
3.58
3.57
3.38
3.36
3.35
3.34
3.33
3.17
3.14
3.13
3.10
2.96
2.94
2.94
2.92
2.92
2.90
2.32
2.04
2.03
1.74
1.72
1.71
1.70
1.69
1.47
1.46
1.44
1.43
N
Ts
O
S
O
3hh
2.01
2.02
2.01
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1.00
2.01
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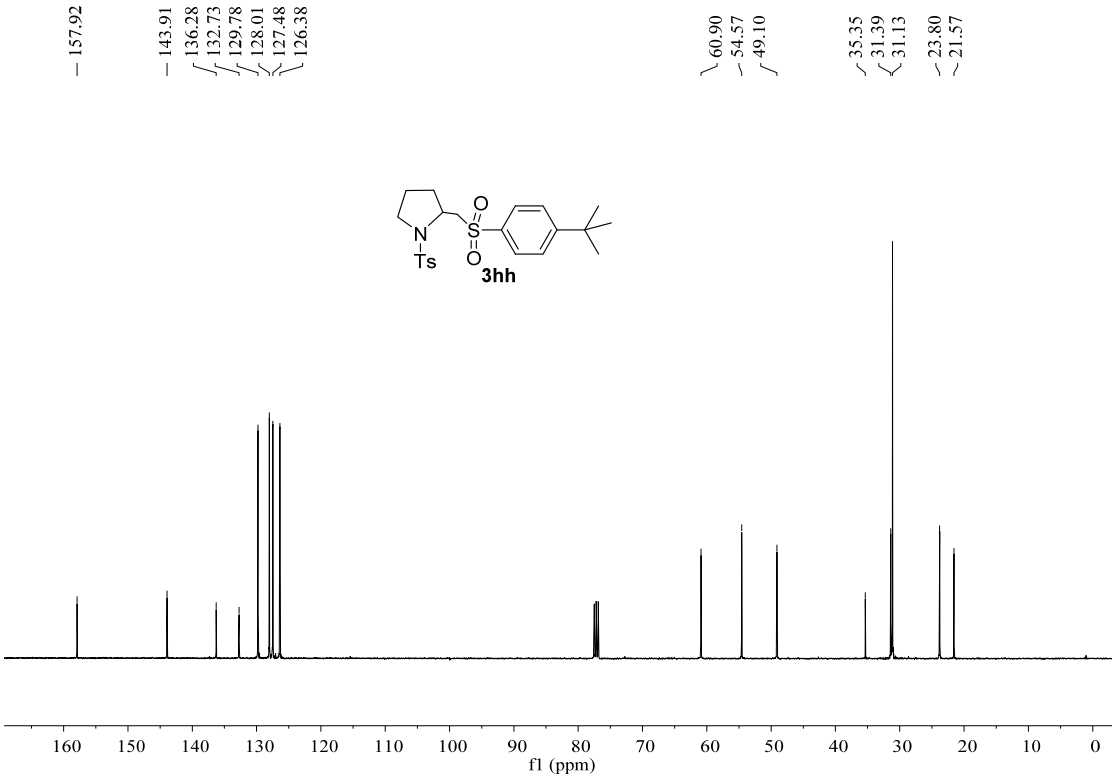
9.00
f1 (ppm)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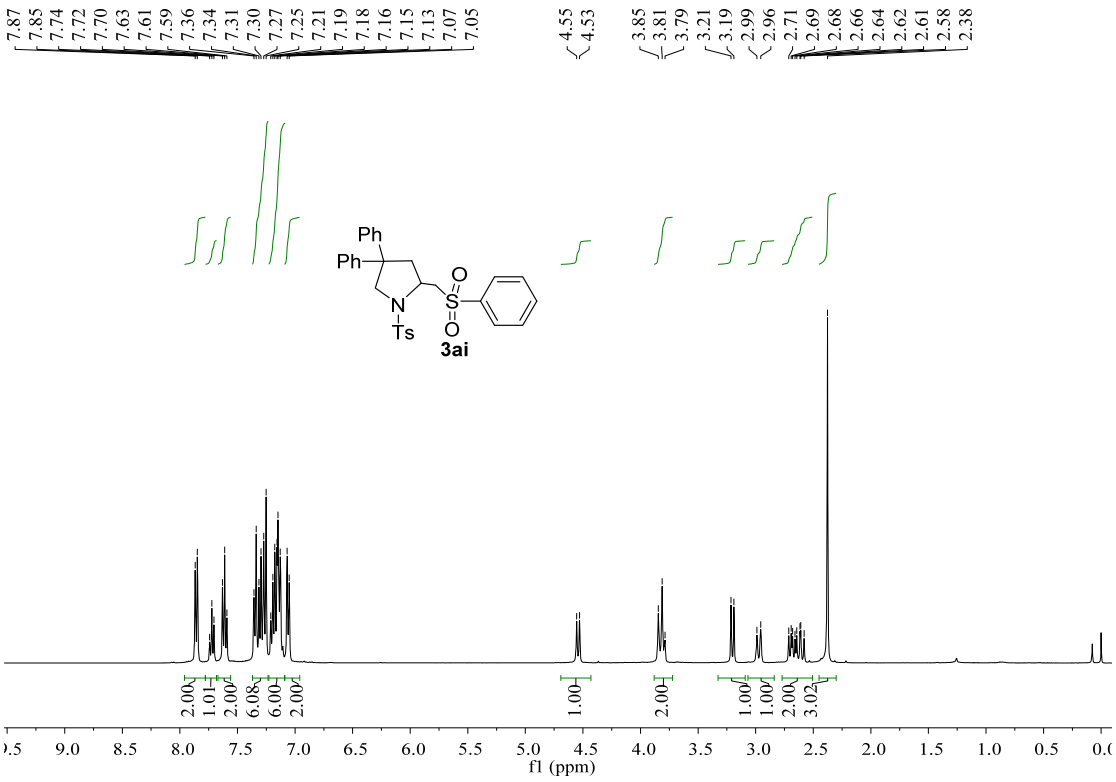
127.48
126.38
60.90
54.57
49.10
35.35
31.39
31.13
23.80
21.57
Ts
3hh
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.31
7.30
7.27
7.25
7.21
7.19
7.18
7.16
7.15
7.13
7.07
7.05
4.55
4.53
3.85
3.81
3.79
3.21
3.19
2.99
2.96
2.71
2.69
2.68
2.66
2.64
2.62
2.61
2.58
2.38
Ph
Ph
Ts
3ai
2.00
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2.00
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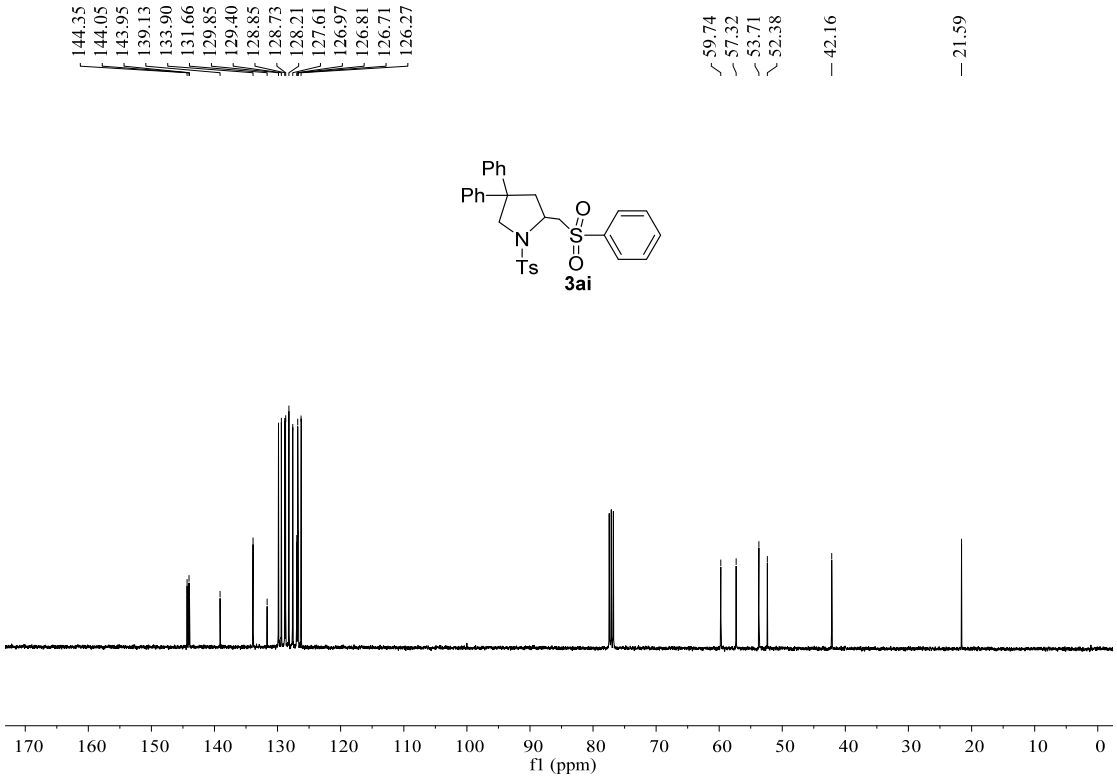
6.00
2.00
1.00
2.00
1.00
1.00
2.00
3.02
f1 (ppm)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129.40
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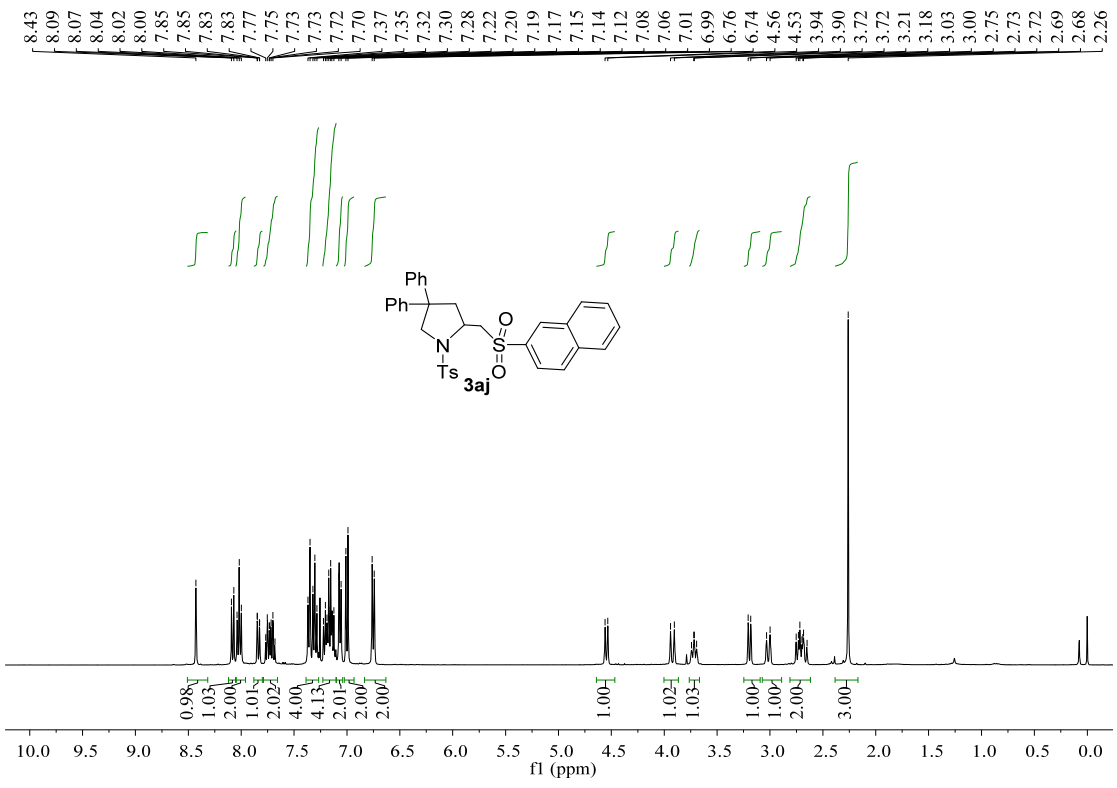
128.73
128.21
127.61
126.97
126.81
126.71
126.27
59.74
57.32
53.71
52.38
42.16
21.59
Ph
Ph
N
Ts
O
S
O
3ai
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.72
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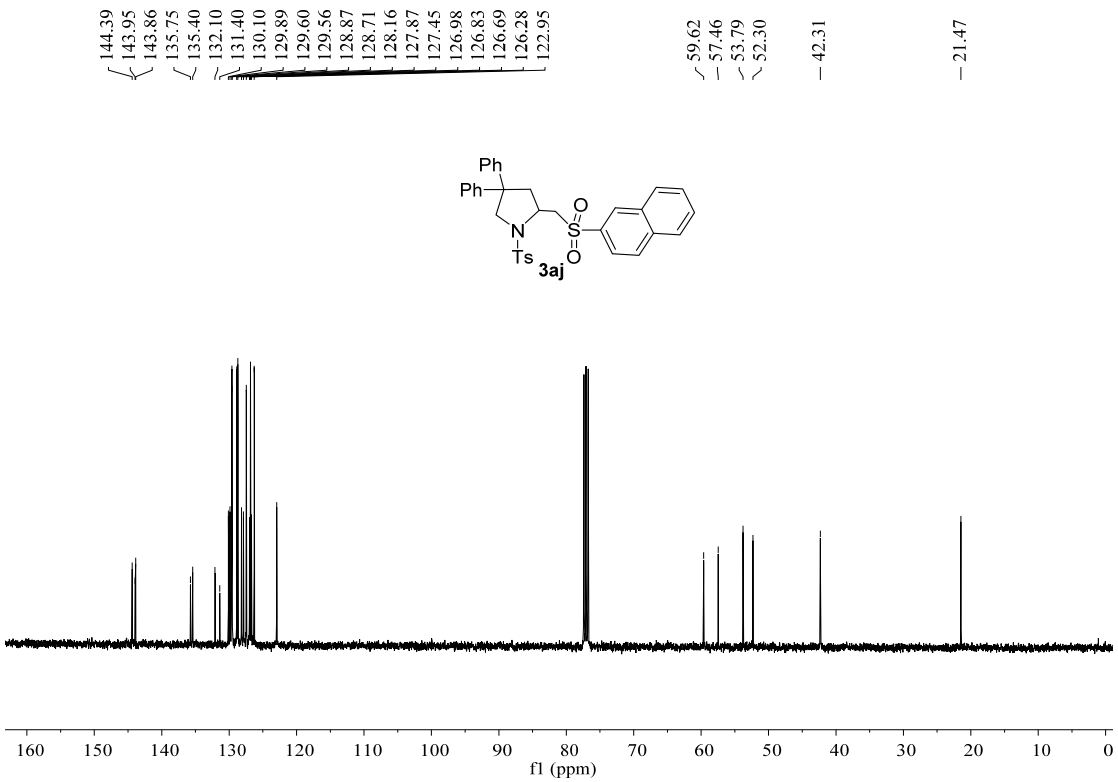
7.28
7.22
7.20
7.19
7.17
7.15
7.14
7.12
7.08
7.06
7.01
6.99
6.76
6.74
4.56
4.53
3.94
3.90
3.72
3.72
3.21
3.18
3.03
3.00
2.75
2.73
2.72
2.69
2.68
2.26
Ph
Ph
N
Ts
O
S
O
3aj
0.98
1.03
2.00
1.01
2.02
4.00
4.13
2.01
2.00
2.00
1.00
1.02
1.03
1.00
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.87
127.45
126.98
126.83
126.69
126.28
122.95
59.62
57.46
53.79
52.30
42.31
21.47
Ph
Ph
N
Ts
O
S
O
3aj
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90
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70
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50
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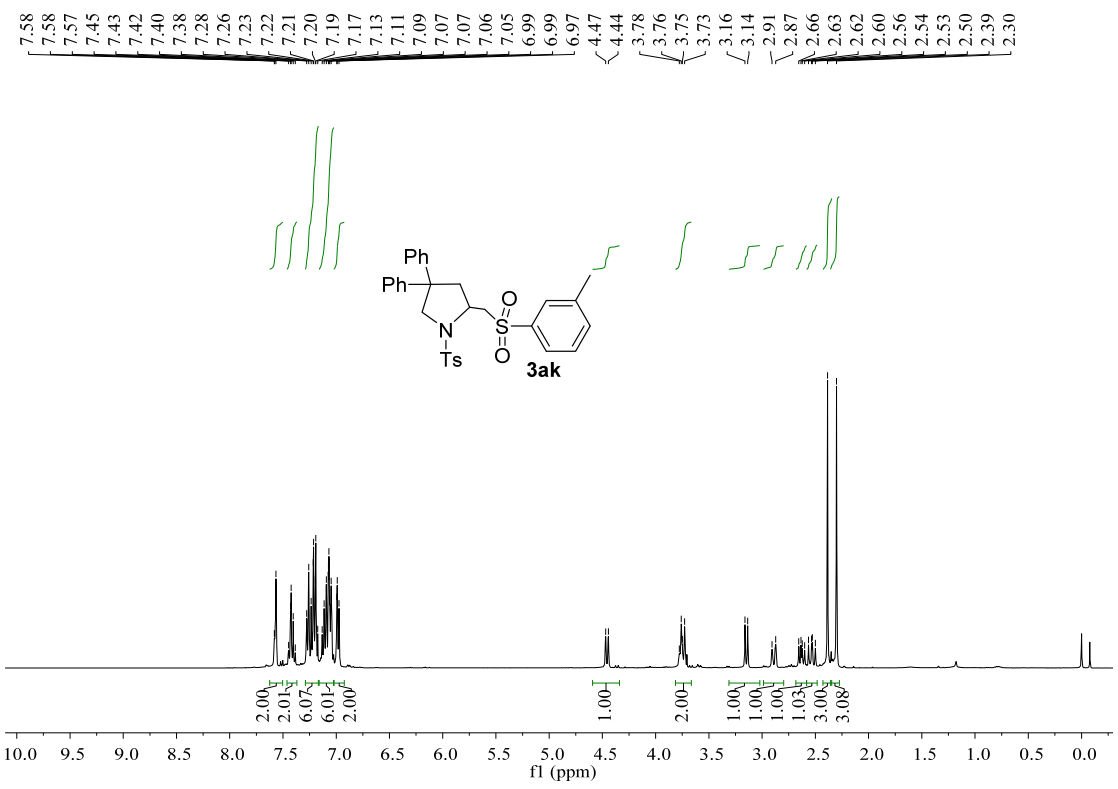
10
0
f1 (ppm)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7.17
7.13
7.11
7.09
7.07
7.07
7.06
7.05
6.99
6.99
6.97
4.47
4.44
3.78
3.76
3.75
3.73
3.16
3.14
2.91
2.87
2.66
2.63
2.62
2.60
2.56
2.54
2.53
2.50
2.39
2.30
Ph
Ph
N
Ts
O
S
O
3ak
2.00
2.01
6.07
6.01
2.00
1.00
2.00
1.00
1.00
1.03
3.00
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.5
2.0
1.5
1.0
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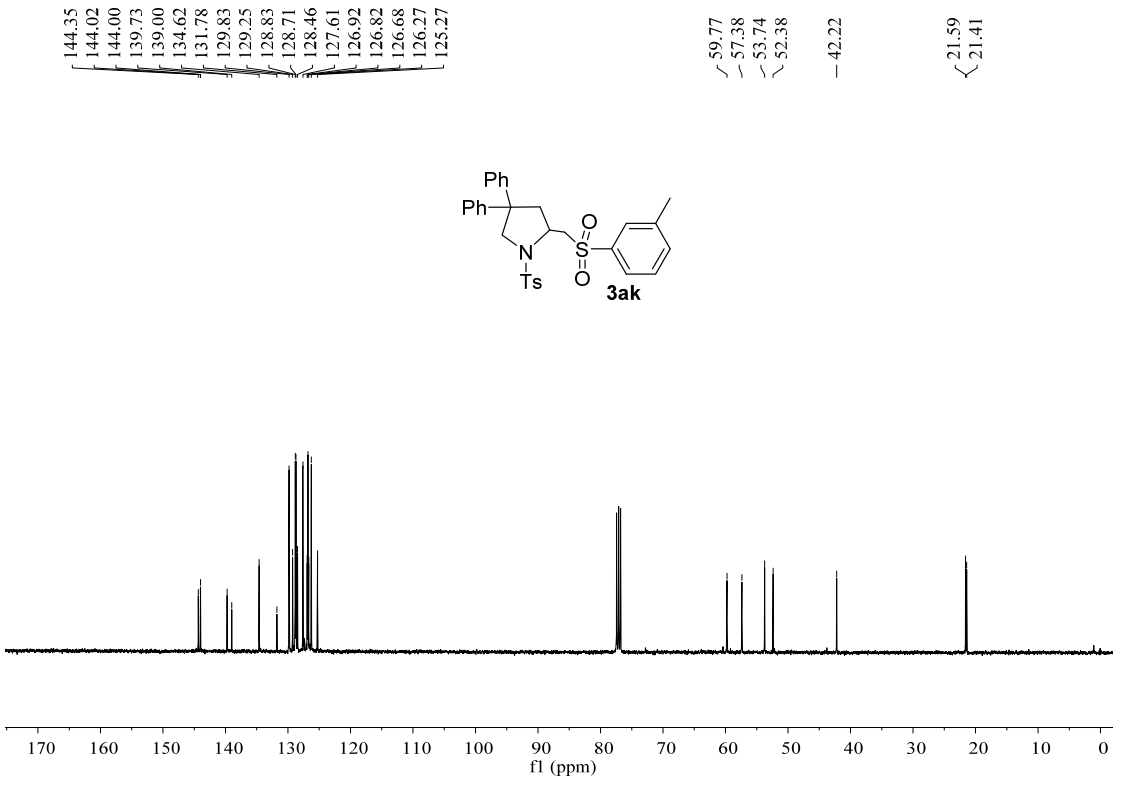
0.0
f1 (ppm)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126.68
126.27
125.27
59.77
57.38
53.74
52.38
42.22
21.59
21.41
Ph
Ph
N
Ts
O
S
O
3ak
170
160
150
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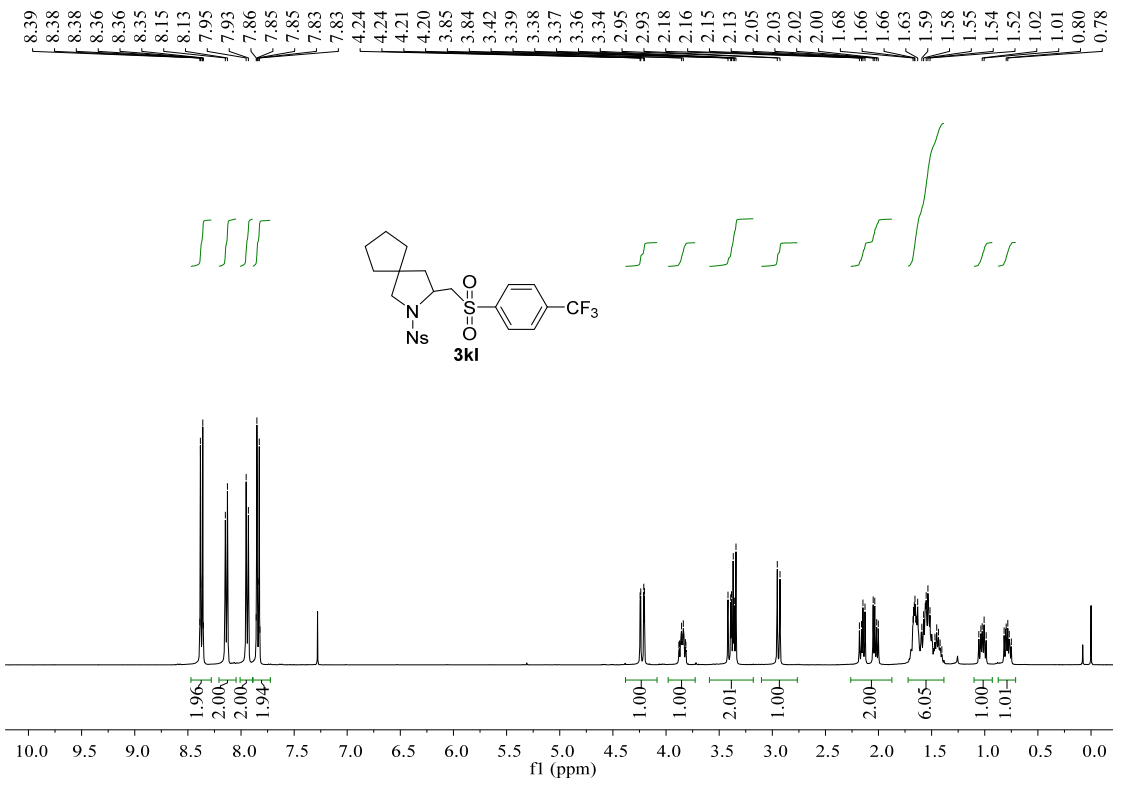
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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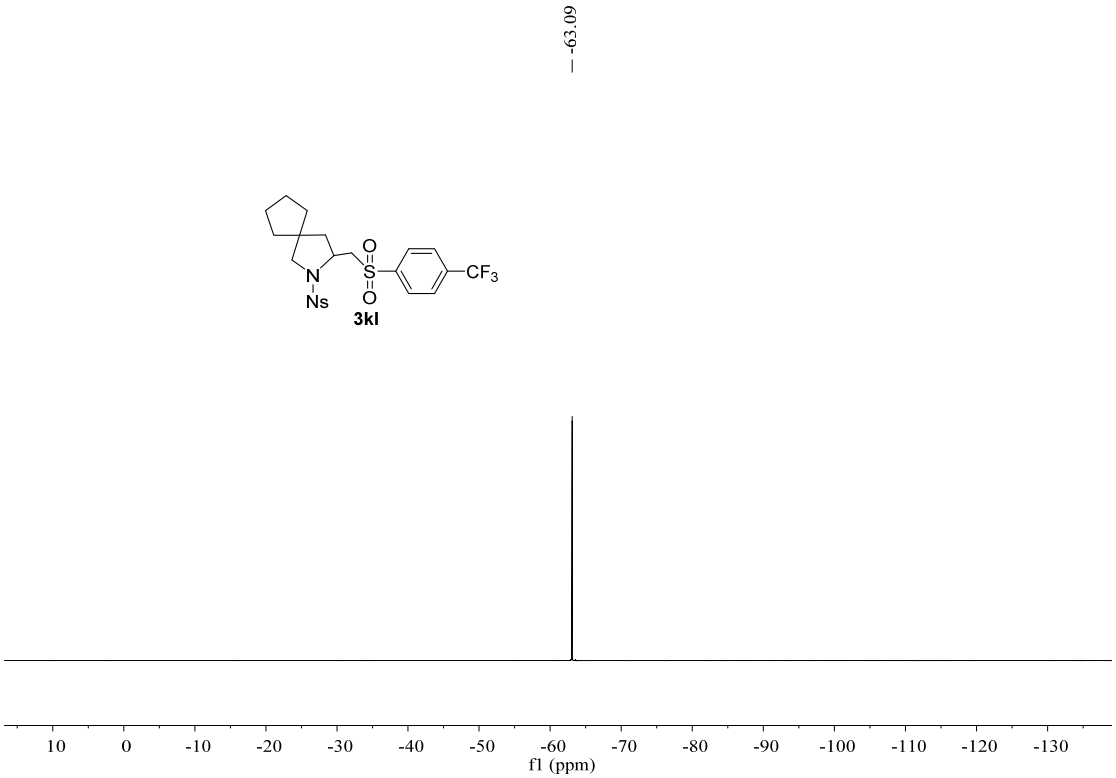
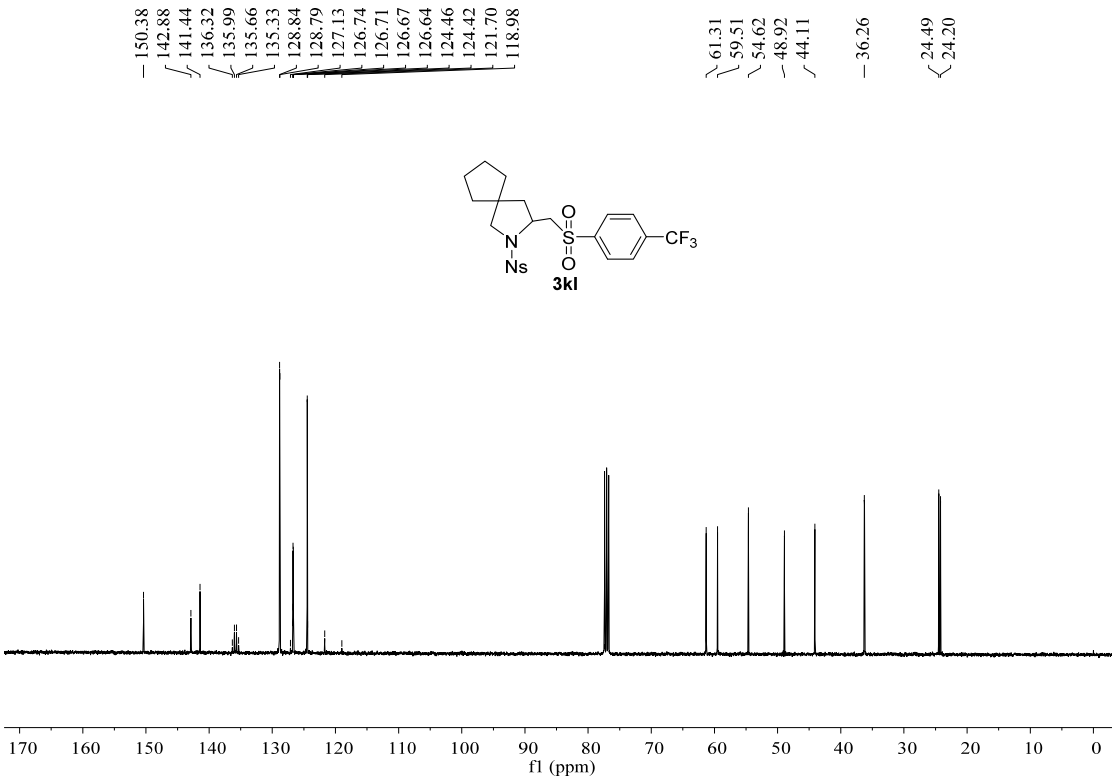
7.85
7.85
7.83
7.83
4.24
4.21
4.20
3.85
3.84
3.42
3.39
3.38
3.37
3.36
3.34
2.95
2.93
2.18
2.16
2.15
2.13
2.05
2.03
2.02
2.00
1.68
1.66
1.66
1.63
1.59
1.58
1.55
1.54
1.52
1.02
1.01
0.80
0.78
N
Ns
O
S
O
CF3
3kl
1.96
2.00
2.00
1.94
1.00
1.00
2.01
1.00
2.00
6.05
1.00
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-63.09
O
S
O
N
Ns
CF3
3kl
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
f1 (ppm)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126.64
124.46
124.42
121.70
118.98
61.31
59.51
54.62
48.92
44.11
36.26
24.49
24.20
O
S
O
N
Ns
CF3
3kl
170
160
150
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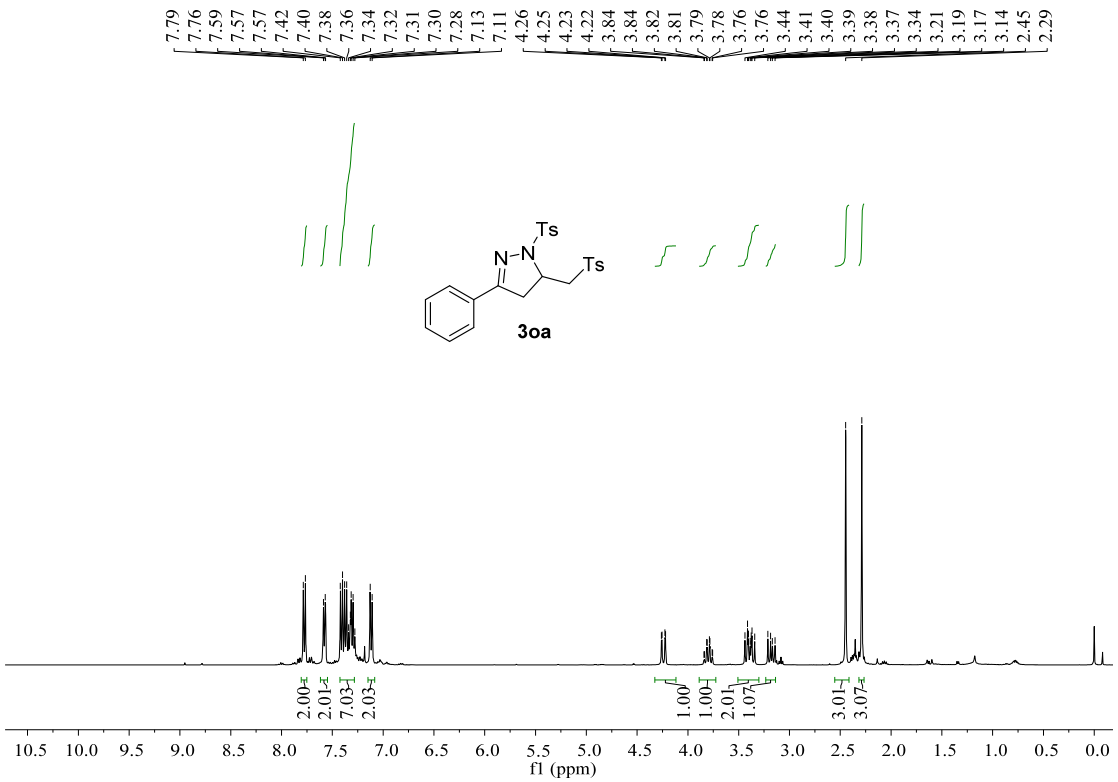
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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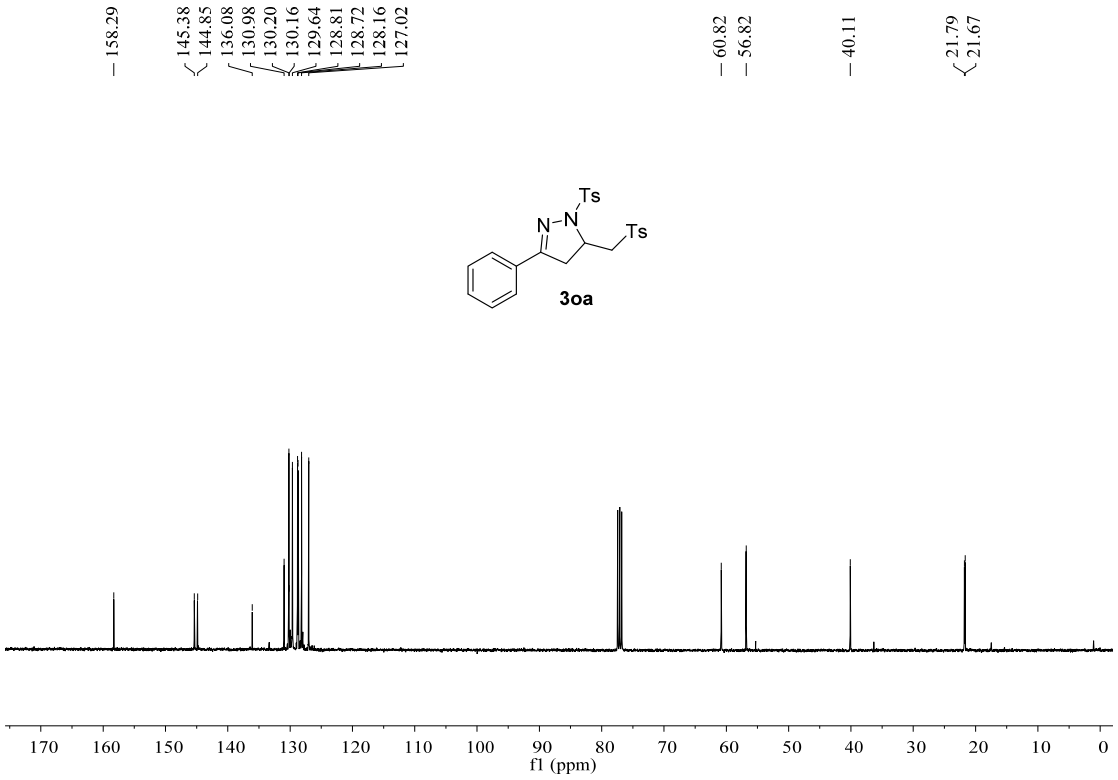
7.34
7.32
7.31
7.30
7.28
7.13
7.11
4.26
4.25
4.23
4.22
3.84
3.84
3.82
3.81
3.79
3.78
3.76
3.76
3.44
3.41
3.40
3.39
3.38
3.37
3.34
3.21
3.19
3.17
3.14
2.45
2.29
Ts
N
N
Ts
3oa
2.00
2.01
7.03
2.03
1.00
1.00
2.01
1.07
3.01
3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.20
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128.81
128.72
128.16
127.02
60.82
56.82
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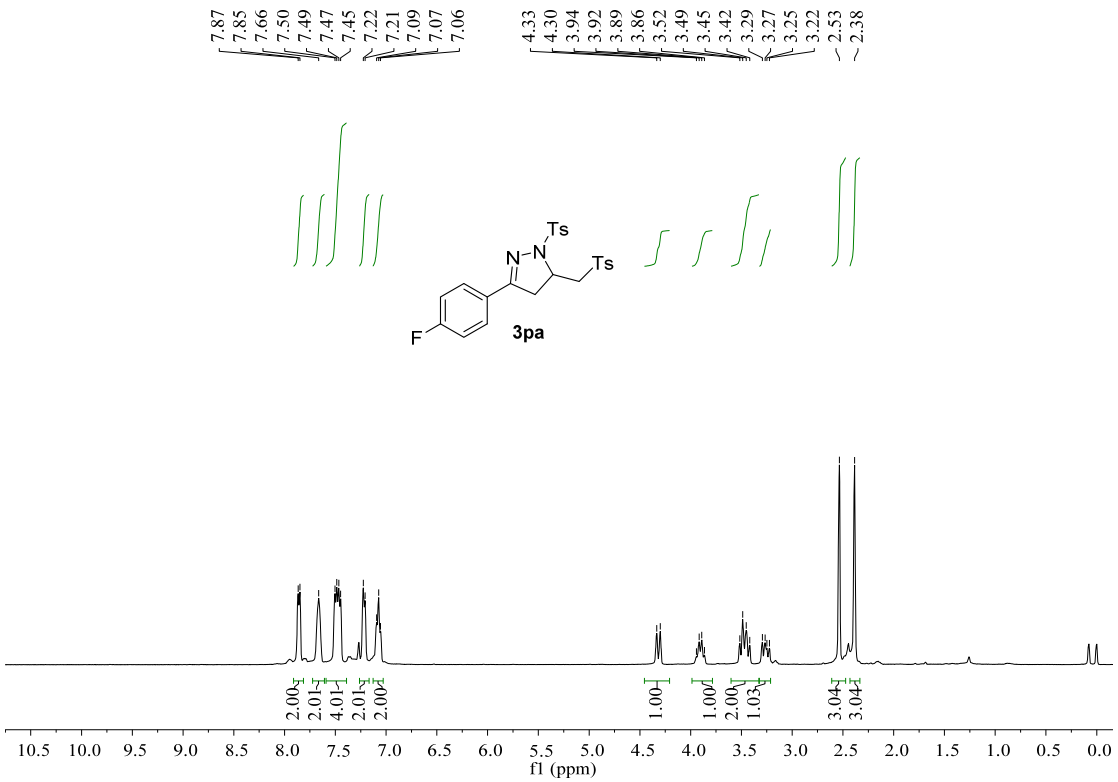
21.67
Ts
N
N
Ts
3oa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.21
7.09
7.07
7.06
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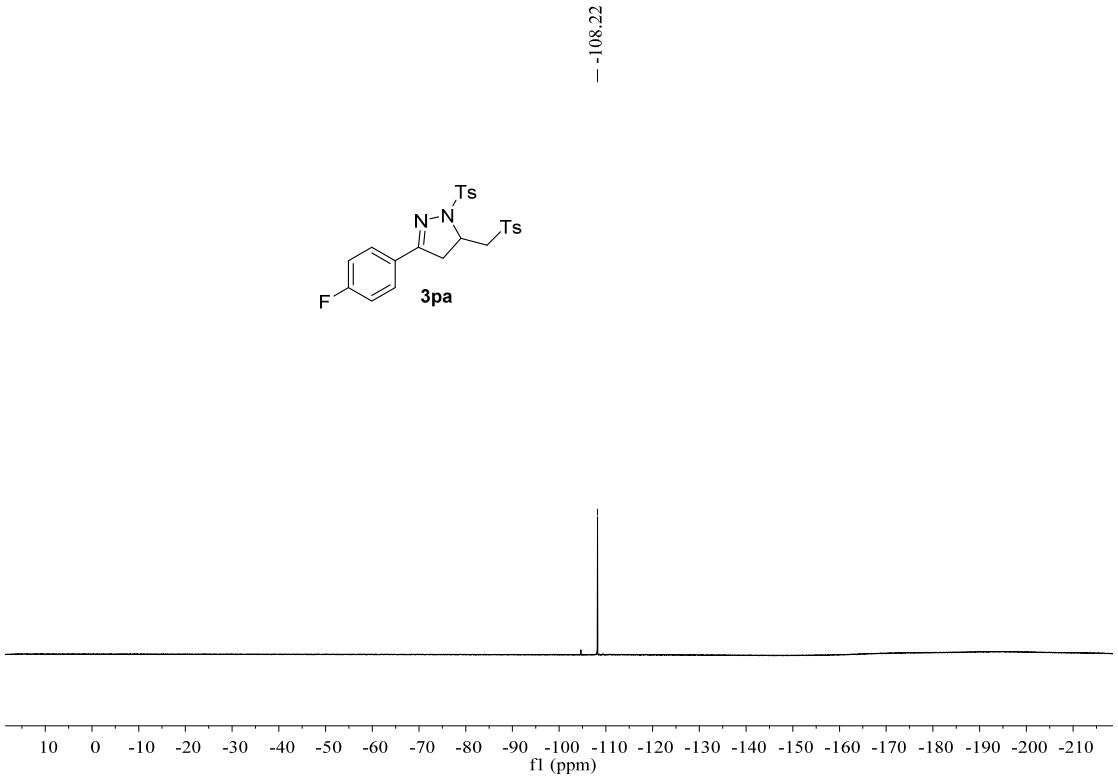
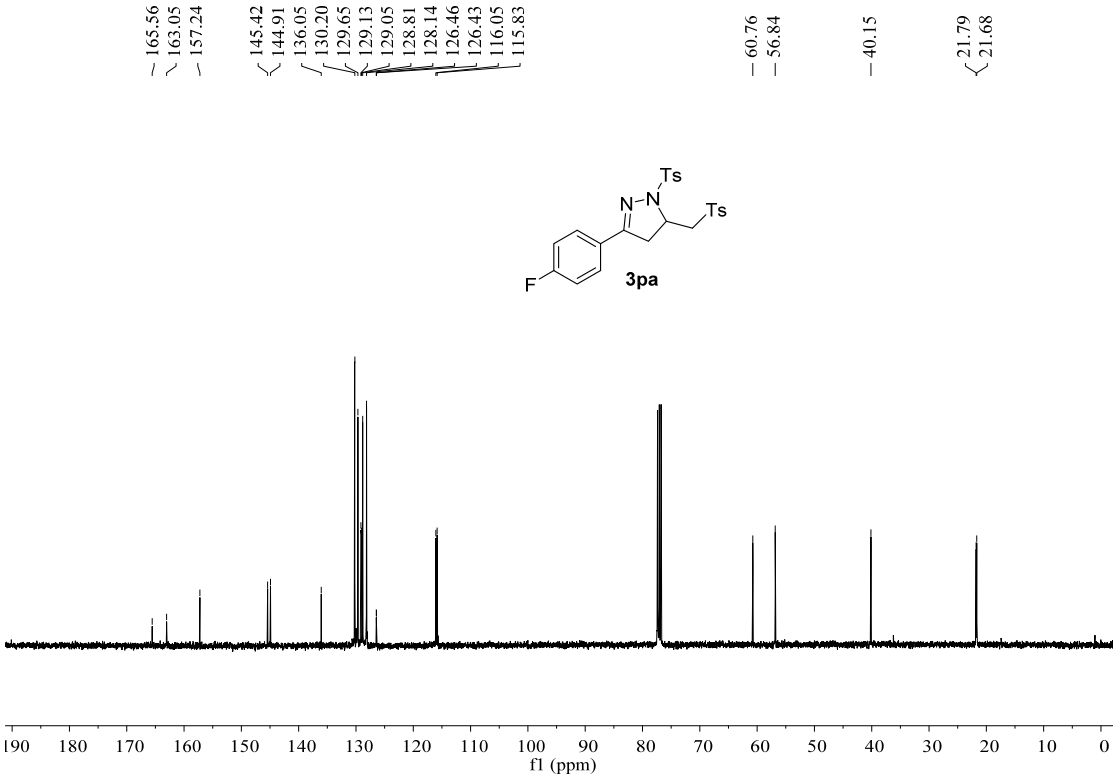
4.30
3.94
3.92
3.89
3.86
3.52
3.49
3.45
3.42
3.29
3.27
3.25
3.22
2.53
2.38
Ts
N
N
Ts
F
3pa
2.00
2.01
4.01
2.01
2.00
1.00
1.00
2.00
1.03
3.04
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-108.22
Ts
N
N
Ts
F
3pa
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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163.05
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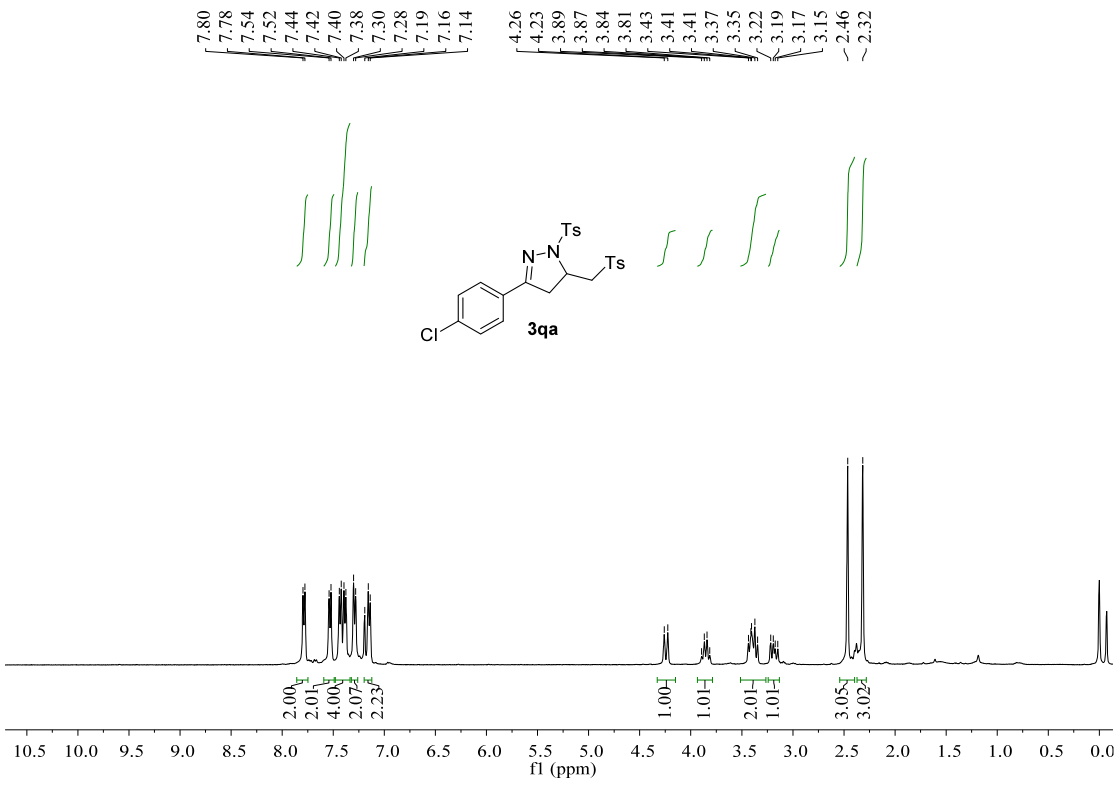
136.05
130.20
129.65
129.13
129.05
128.81
128.14
126.46
126.43
116.05
115.83
60.76
56.84
40.15
21.79
21.68
Ts
N
N
Ts
F
3pa
f1 (ppm)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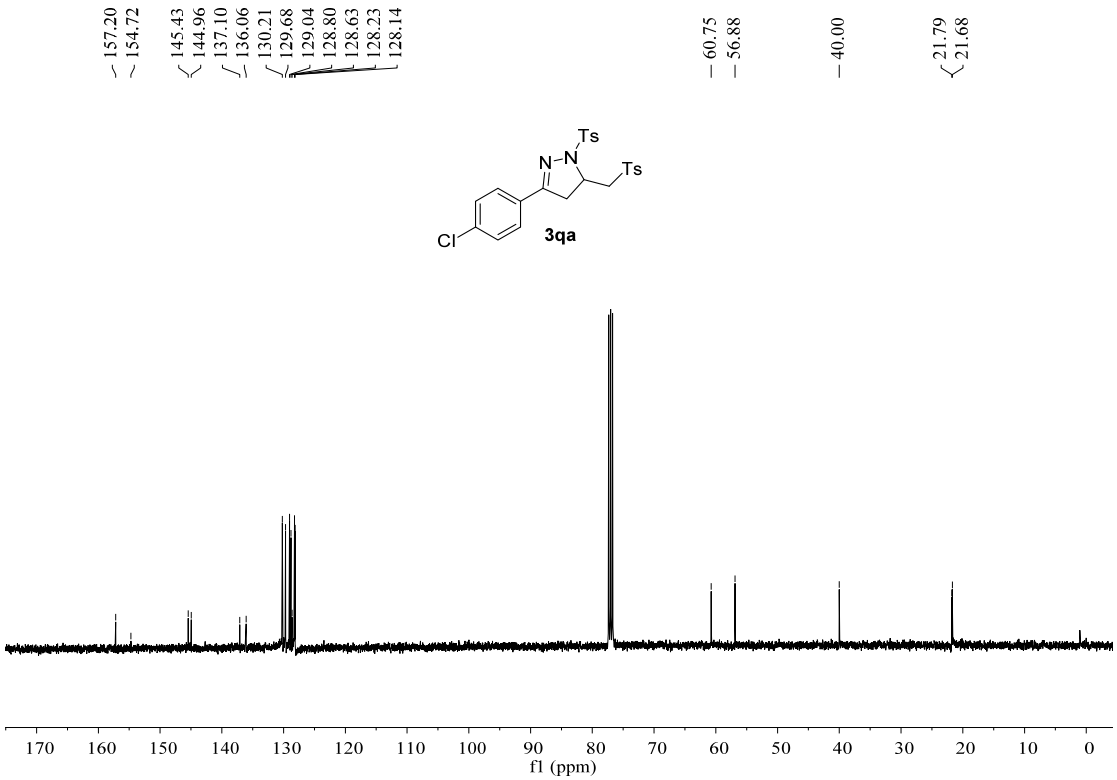
7.38
7.30
7.28
7.19
7.16
7.14
4.26
4.23
3.89
3.87
3.84
3.81
3.43
3.41
3.41
3.37
3.35
3.22
3.19
3.17
3.15
2.46
2.32
Ts
N
N
Ts
Cl
3qa
2.00
2.01
4.00
2.07
2.23
1.00
1.01
2.01
1.01
3.05
3.02
f1 (ppm)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137.10
136.06
130.21
129.68
129.04
128.80
128.63
128.23
128.14
60.75
56.88
40.00
21.79
21.68
Ts
N
N
Ts
Cl
3qa
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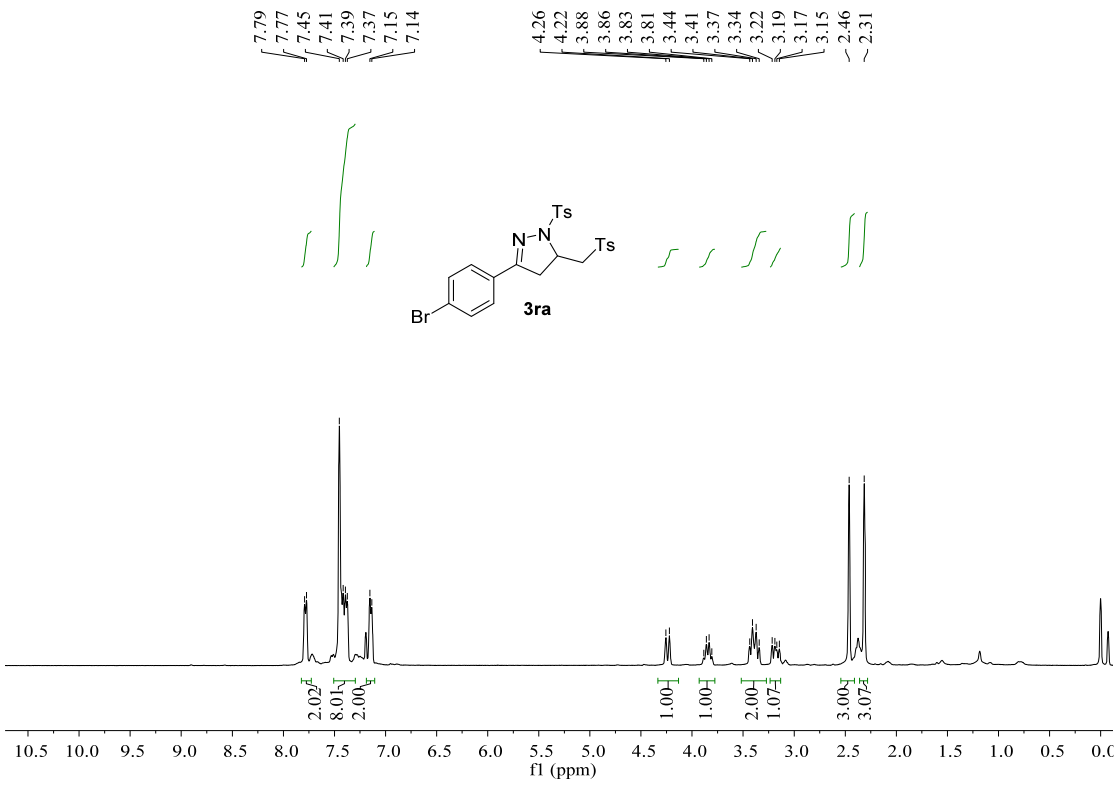
f1 (ppm)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4.22
3.88
3.86
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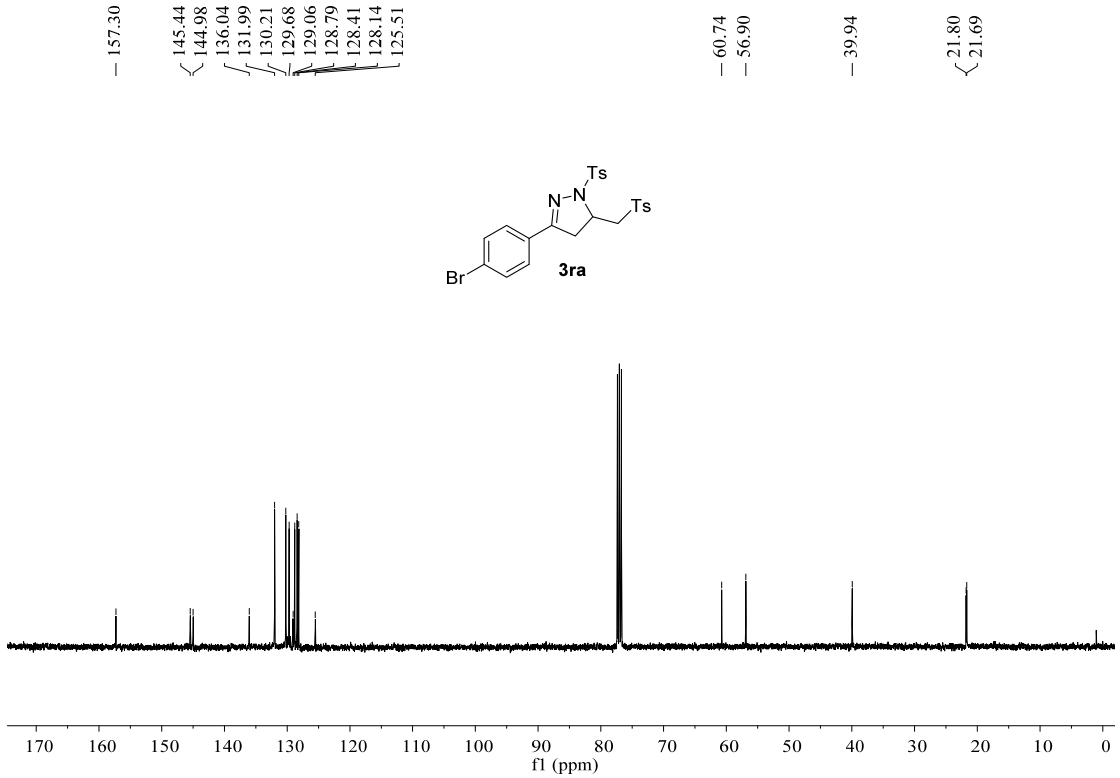
3.81
3.44
3.41
3.37
3.34
3.22
3.19
3.17
3.15
2.46
2.31
Ts
N
N
Ts
Br
3ra
2.02
8.01
2.00
1.00
1.00
2.00
1.07
3.00
3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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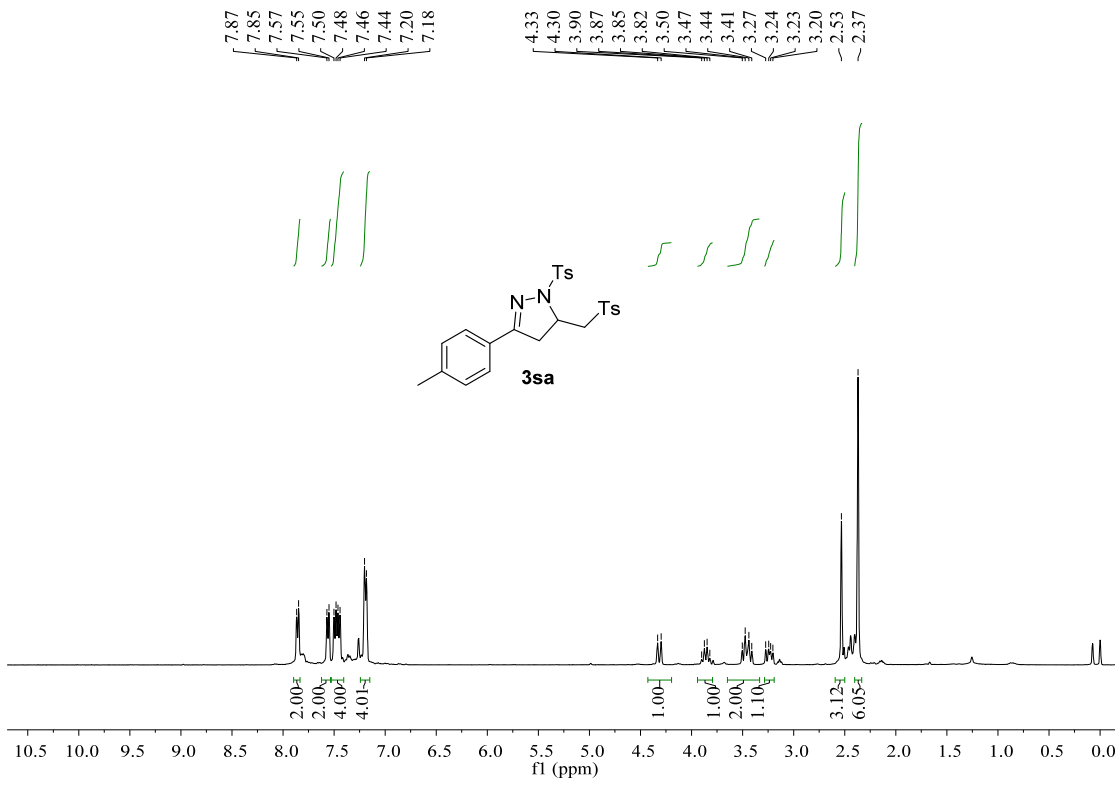
129.68
129.06
128.79
128.41
128.14
125.51
60.74
56.90
39.94
21.80
21.69
Ts
N
N
Ts
Br
3ra
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.44
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7.18
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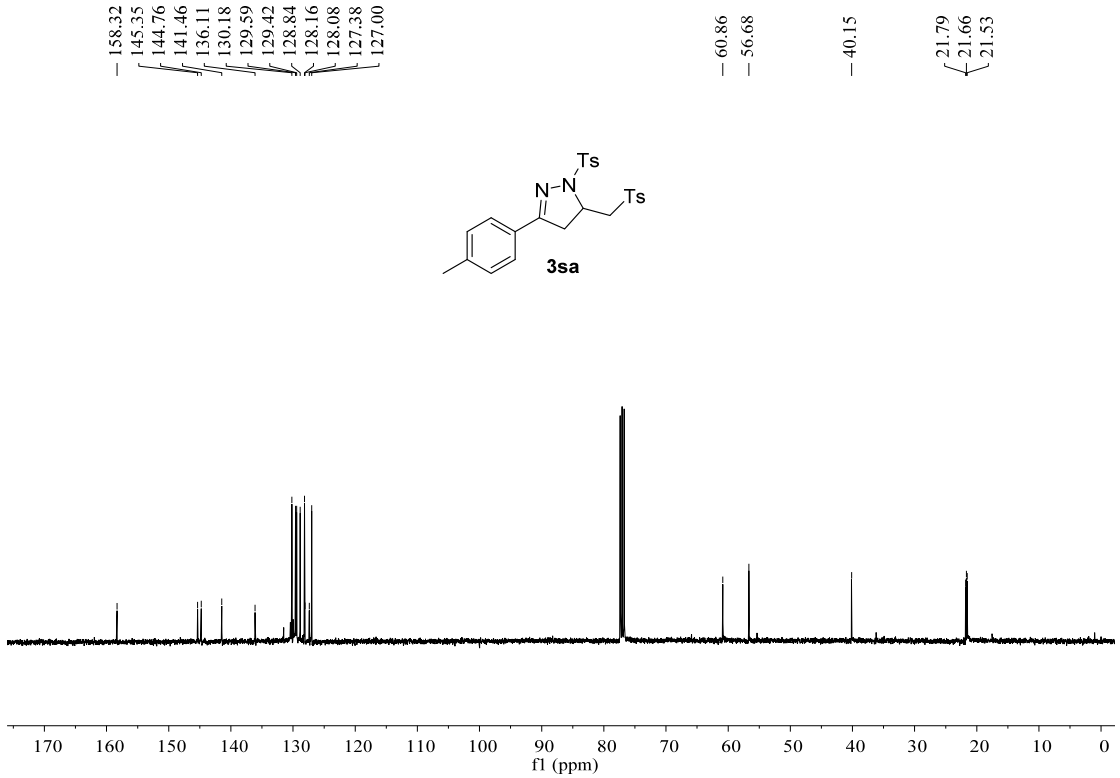
4.30
3.90
3.87
3.85
3.82
3.50
3.47
3.44
3.41
3.27
3.24
3.23
3.20
2.53
2.37
Ts
N
N
Ts
3sa
2.00
2.00
4.00
4.01
1.00
1.00
2.00
1.10
3.12
6.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.42
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128.16
128.08
127.38
127.00
60.86
56.68
40.15
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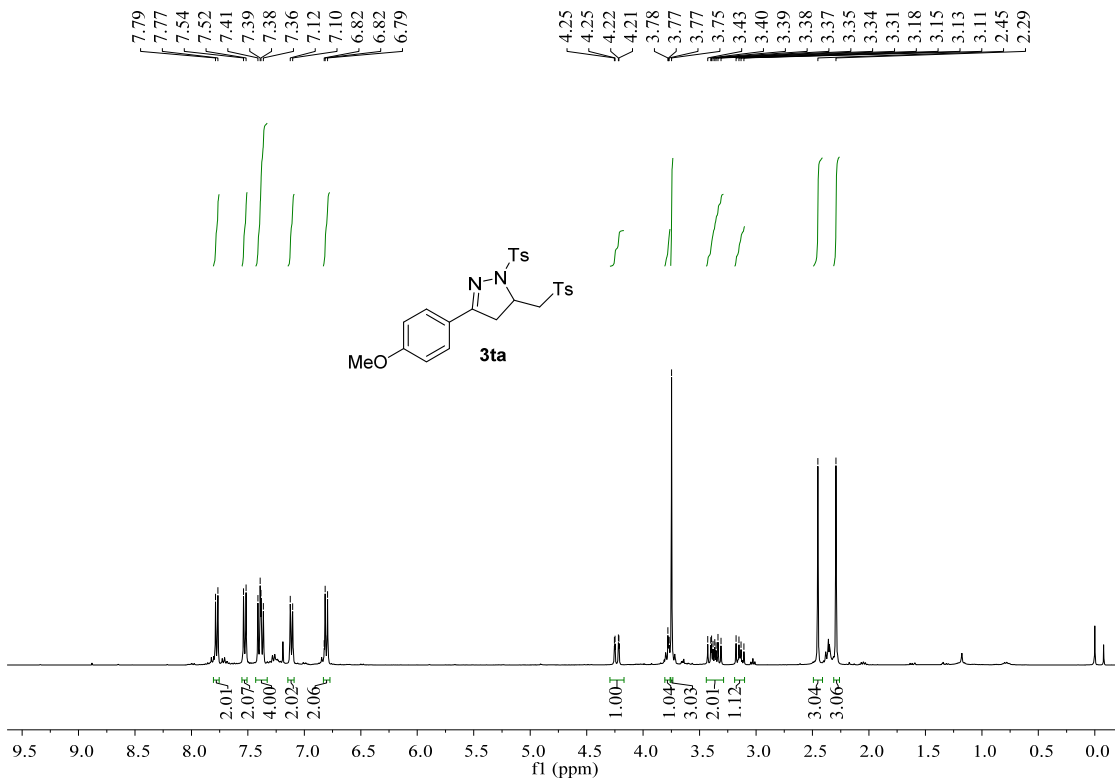
21.53
Ts
N
N
Ts
3sa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.10
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6.79
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4.25
4.22
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3.77
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3.40
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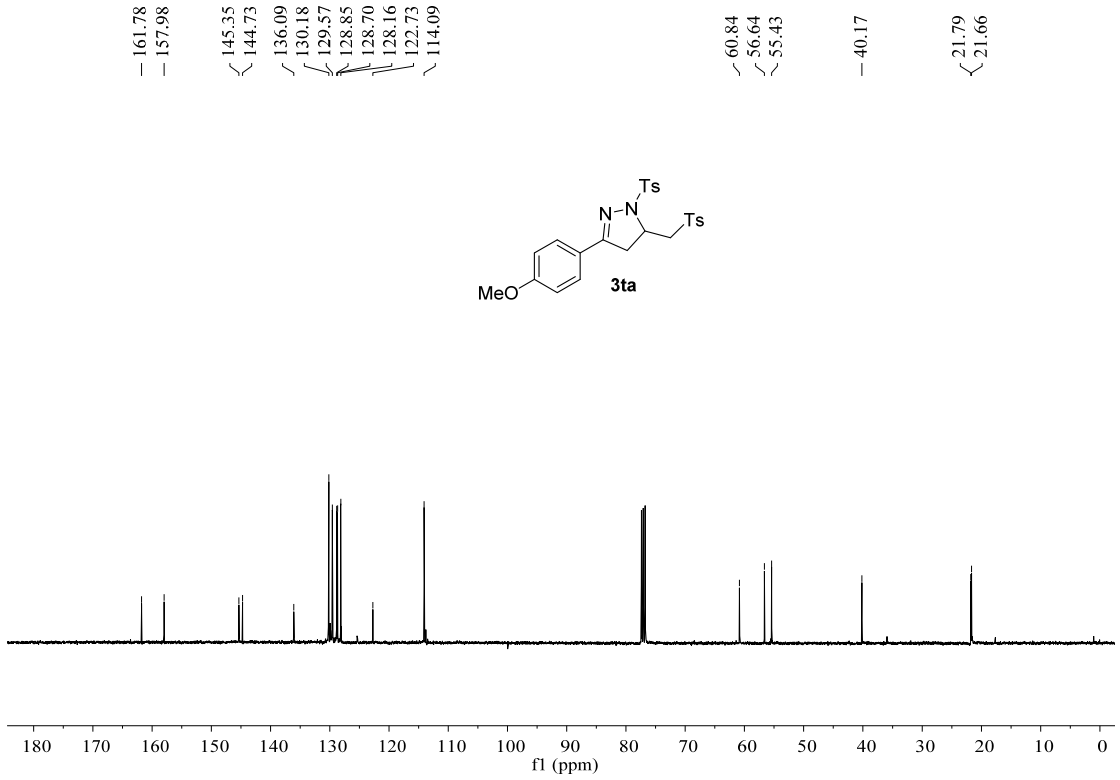
3.38
3.37
3.35
3.34
3.31
3.18
3.15
3.13
3.11
2.45
2.29
Ts
N
N
Ts
MeO
3ta
2.01
2.07
4.00
2.02
2.06
1.00
1.04
3.03
2.01
1.12
3.04
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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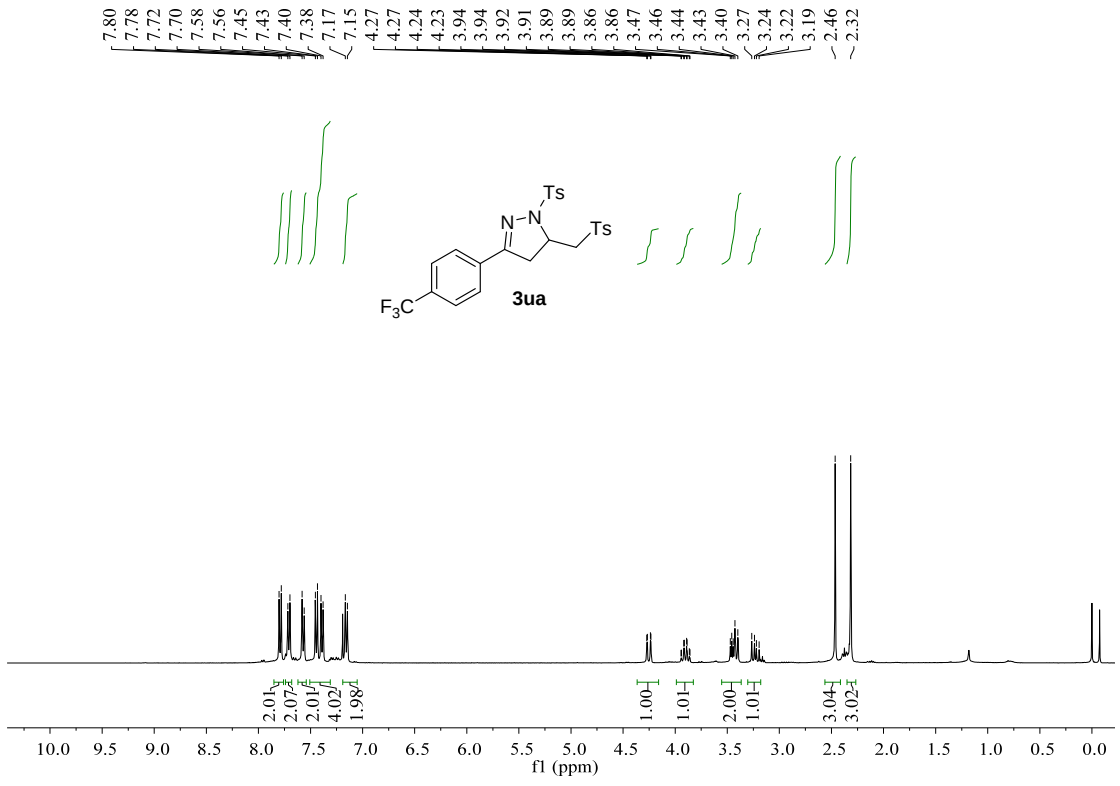
128.85
128.70
128.16
122.73
114.09
60.84
56.64
55.43
40.17
21.79
21.66
Ts
N
N
Ts
MeO
3ta
f1 (ppm)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7.70
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7.56
7.45
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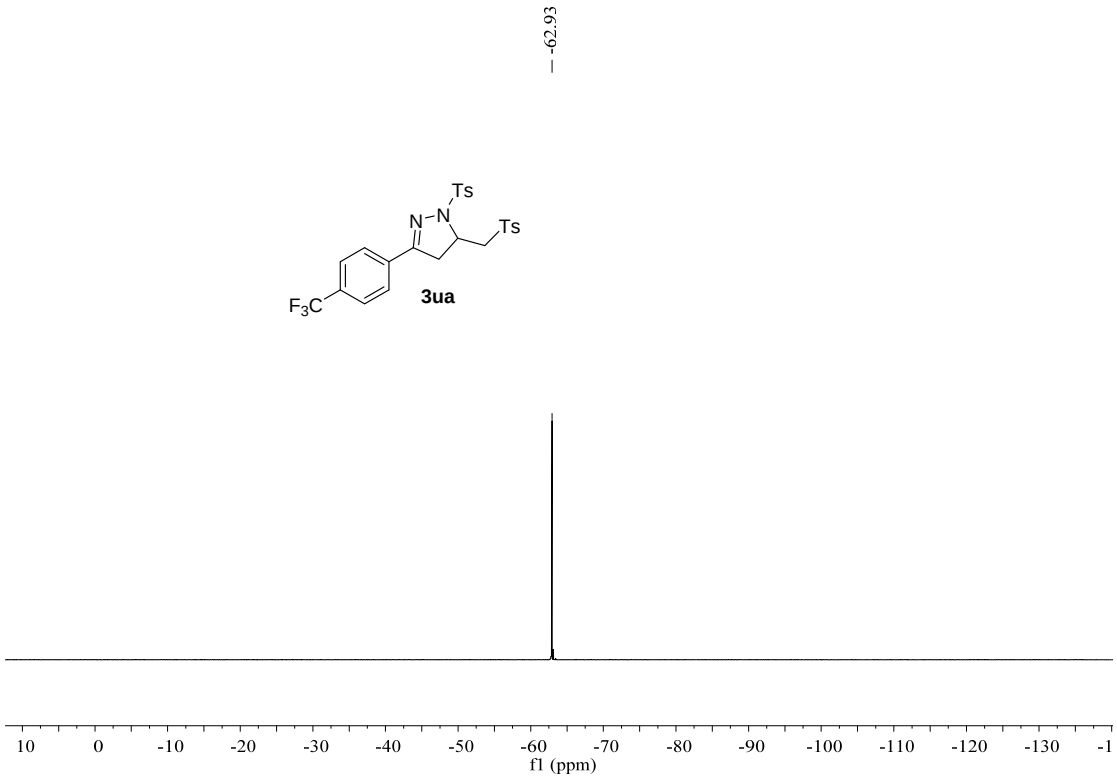
7.38
7.17
7.15
4.27
4.27
4.24
4.23
3.94
3.94
3.92
3.91
3.89
3.89
3.86
3.86
3.47
3.46
3.44
3.43
3.40
3.27
3.24
3.22
3.19
2.46
2.32
Ts
N
N
Ts
F3C
3ua
2.01
2.07
2.01
4.02
1.98
1.00
1.01
2.00
1.01
3.04
3.02
f1 (ppm)


-62.93
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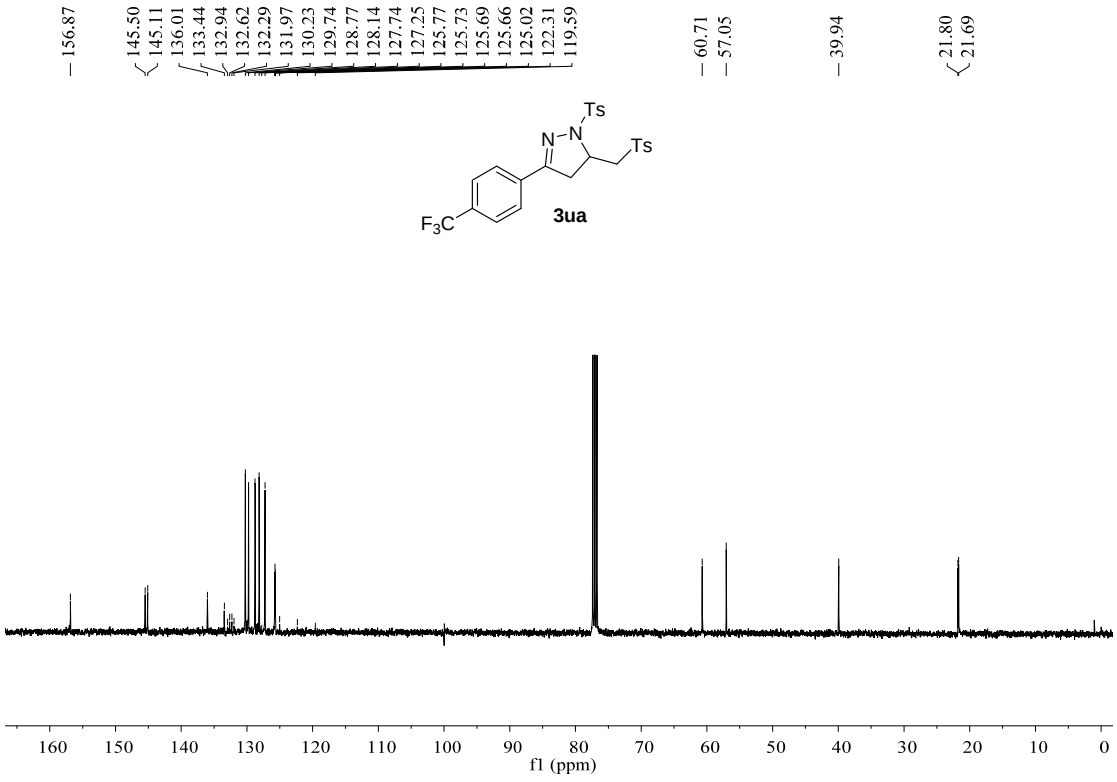
N
N
Ts
F3C
3ua
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -1
f1 (ppm)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129.74
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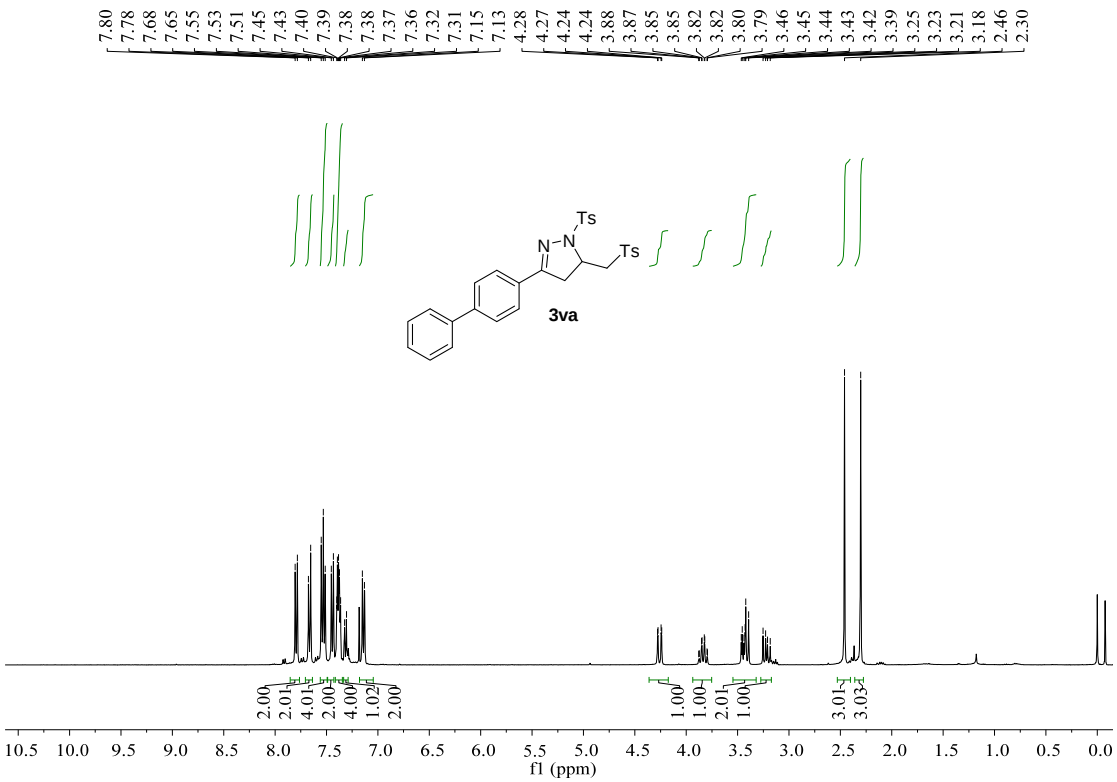
128.14
127.74
127.25
125.77
125.73
125.69
125.66
125.02
122.31
119.59
60.71
57.05
39.94
21.80
21.69
Ts
N
N
Ts
F3C
3ua
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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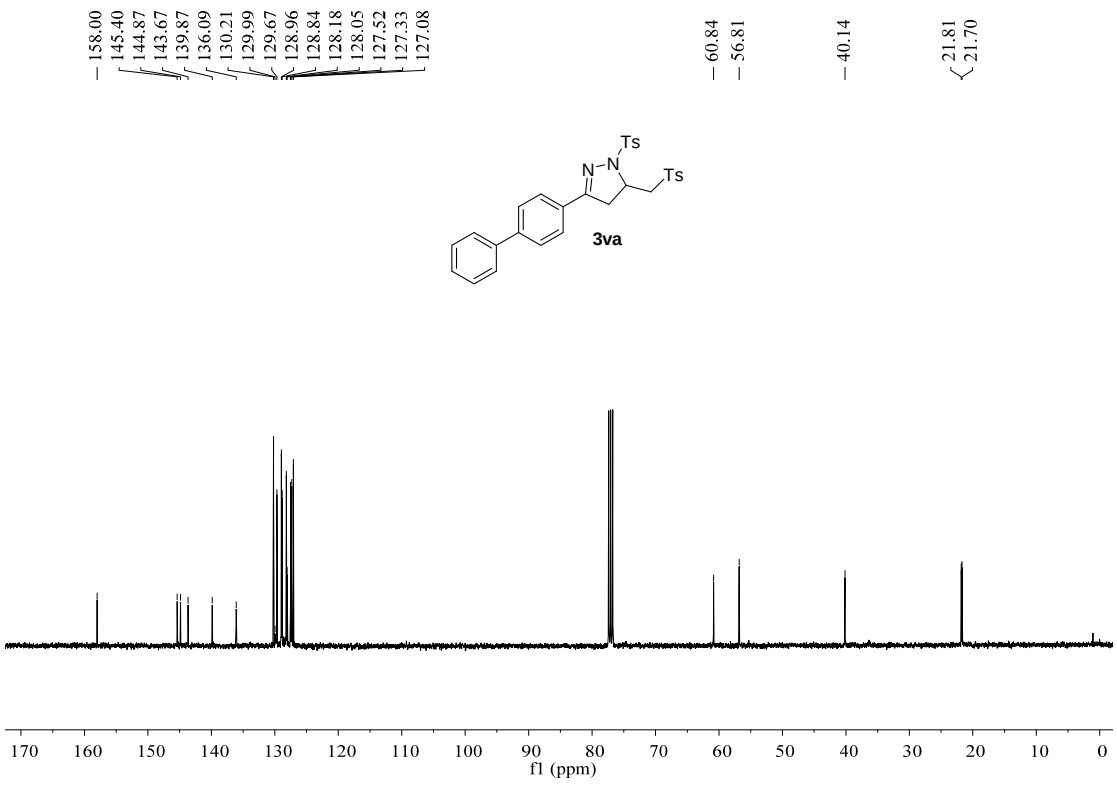
7.53
7.51
7.45
7.43
7.40
7.39
7.38
7.38
7.37
7.36
7.32
7.31
7.15
7.13
4.28
4.27
4.24
4.24
3.88
3.87
3.85
3.85
3.82
3.82
3.80
3.79
3.46
3.45
3.44
3.43
3.42
3.39
3.25
3.23
3.21
3.18
2.46
2.30
Ts
N
N
Ts
3va
2.00
2.01
4.01
2.00
4.00
1.02
2.00
1.00
1.00
2.01
1.00
3.01
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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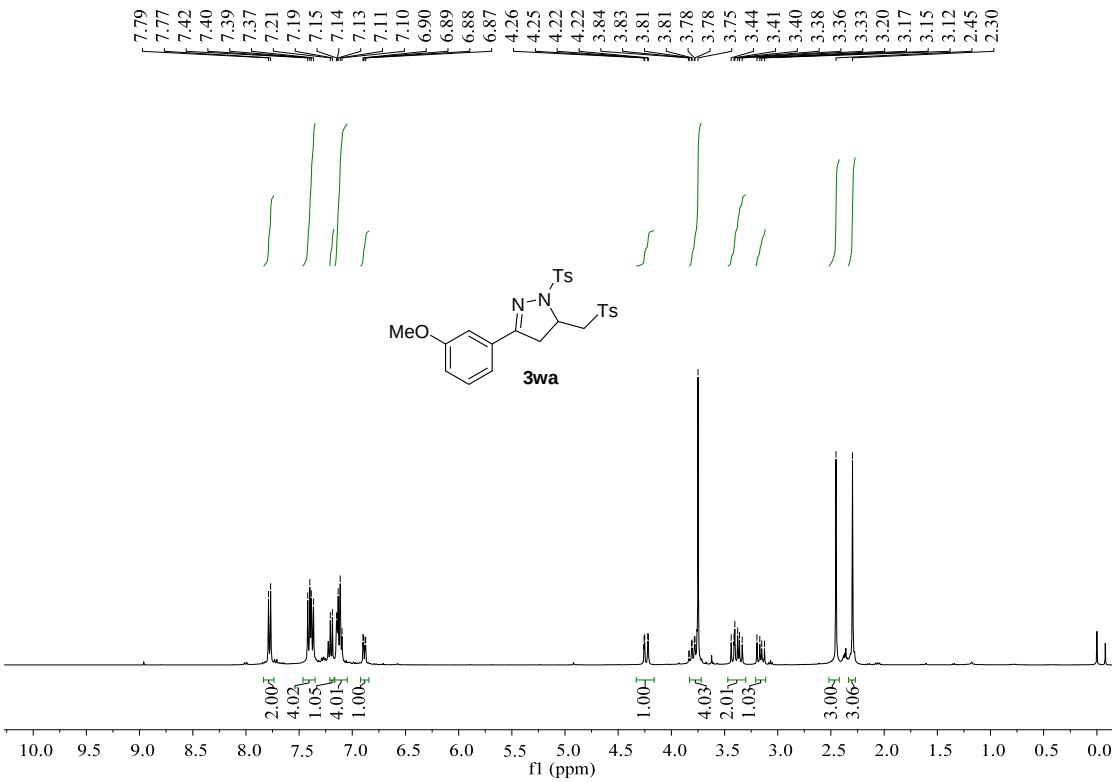
128.96
128.84
128.18
128.05
127.52
127.33
127.08
60.84
56.81
40.14
21.81
21.70
Ts
N
N
Ts
3va
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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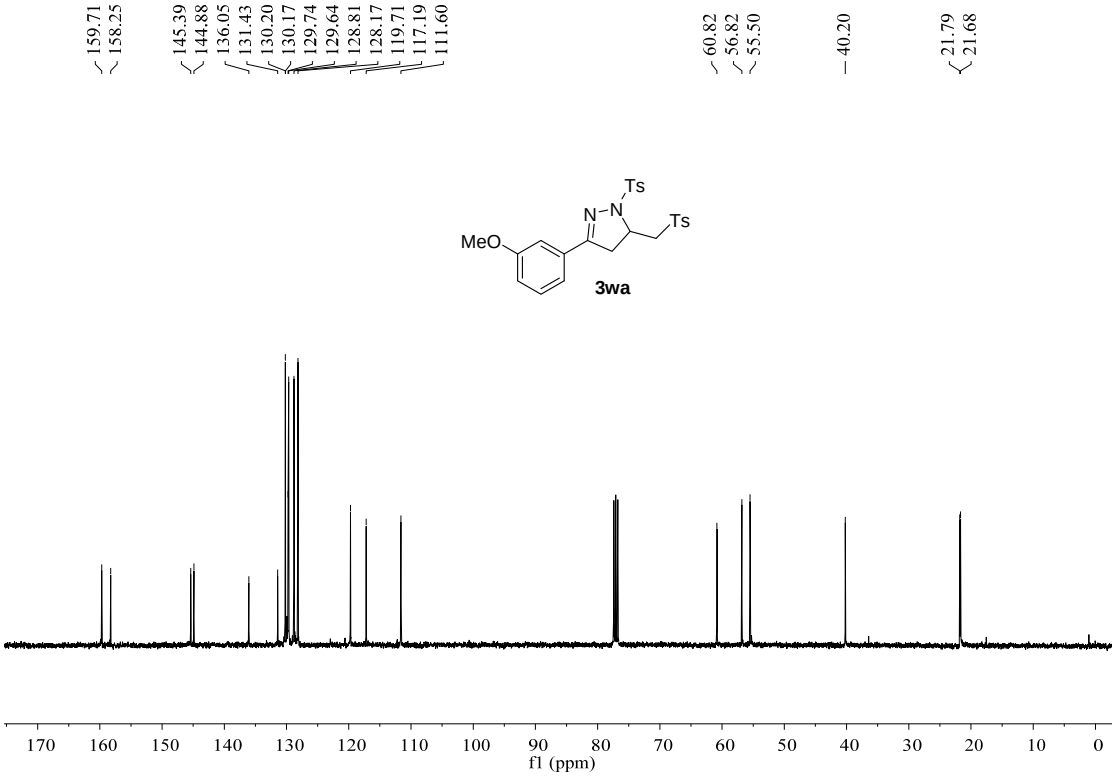
7.19
7.15
7.14
7.13
7.11
7.10
6.90
6.89
6.88
6.87
4.26
4.25
4.22
4.22
3.84
3.83
3.81
3.81
3.78
3.78
3.75
3.44
3.41
3.40
3.38
3.36
3.33
3.20
3.17
3.15
3.12
2.45
2.30
Ts
N
N
Ts
MeO
3wa
2.00
4.02
1.05
4.01
1.00
1.00
4.03
2.01
1.03
3.00
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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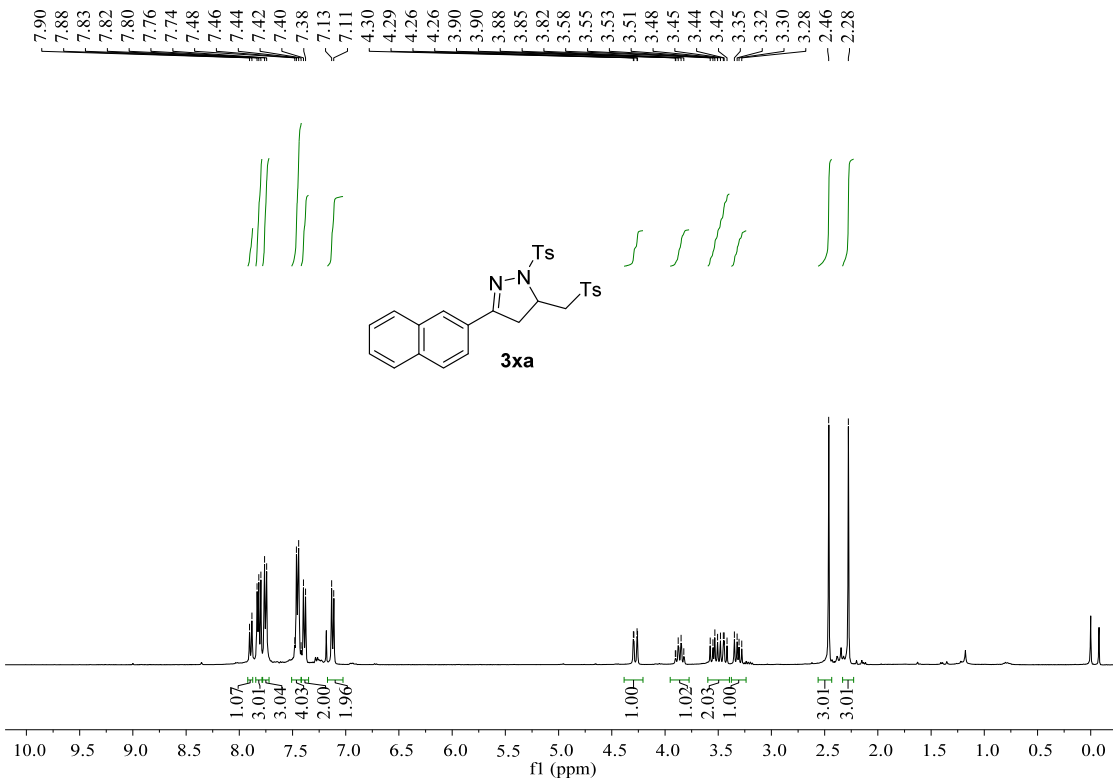
136.05
131.43
130.20
130.17
129.74
129.64
128.81
128.17
119.71
117.19
111.60
60.82
56.82
55.50
40.20
21.79
21.68
Ts
N
N
Ts
MeO
3wa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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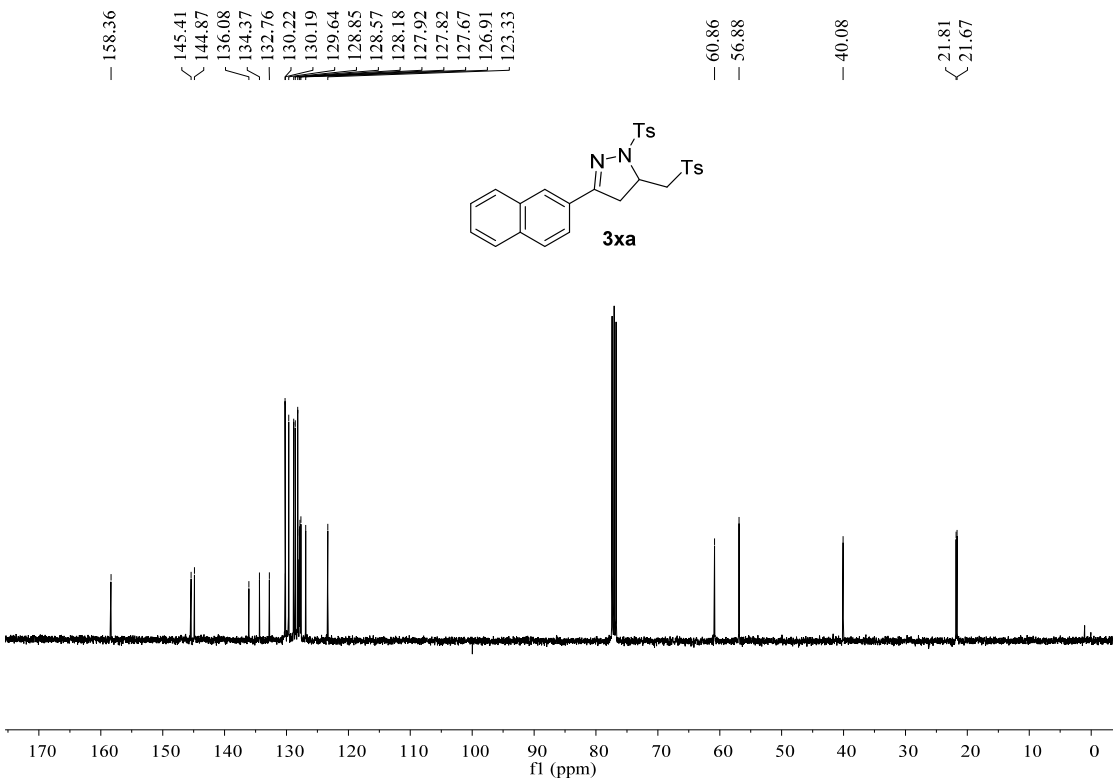
7.76
7.74
7.48
7.46
7.44
7.42
7.40
7.38
7.13
7.11
4.30
4.29
4.26
4.26
3.90
3.90
3.88
3.85
3.82
3.58
3.55
3.53
3.51
3.48
3.45
3.44
3.42
3.35
3.32
3.30
3.28
2.46
2.28
Ts
N
N
Ts
3xa
1.07
3.01
3.04
4.03
2.00
1.96
1.00
1.02
2.03
1.00
3.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.76
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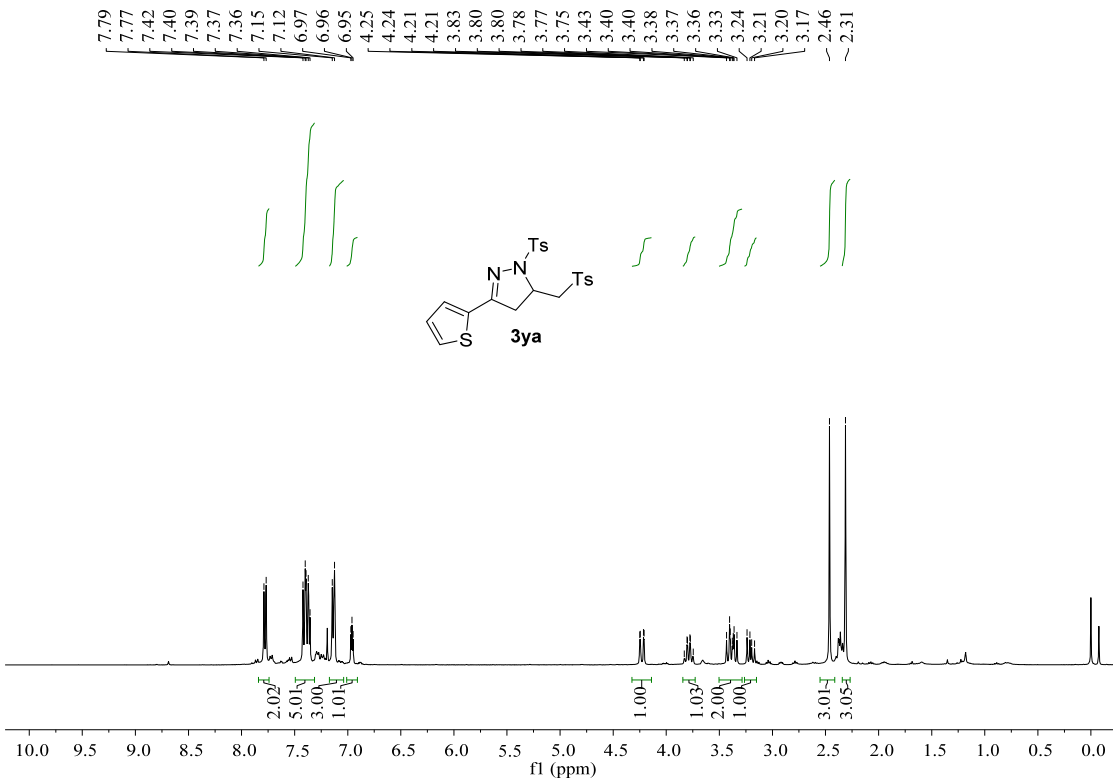
130.19
129.64
128.85
128.57
128.18
127.92
127.82
127.67
126.91
123.33
60.86
56.88
40.08
21.81
21.67
Ts
N
N
Ts
3xa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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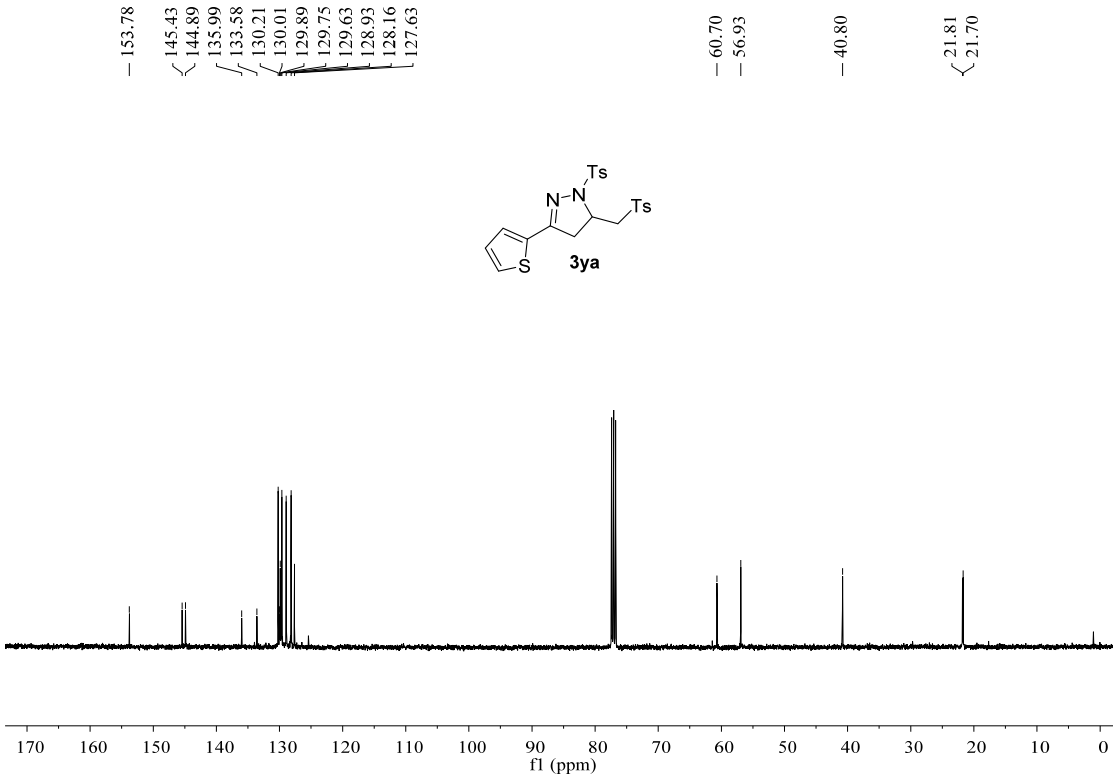
7.15
7.12
6.97
6.96
6.95
4.25
4.24
4.21
4.21
3.83
3.80
3.80
3.78
3.77
3.75
3.43
3.40
3.40
3.38
3.37
3.36
3.33
3.24
3.21
3.20
3.17
2.46
2.31
Ts
N
N
Ts
S
3ya
2.02
5.01
3.00
1.01
1.00
1.03
2.00
1.00
3.01
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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145.43
144.89
135.99
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130.21
130.01
129.89
129.75
129.63
128.93
128.16
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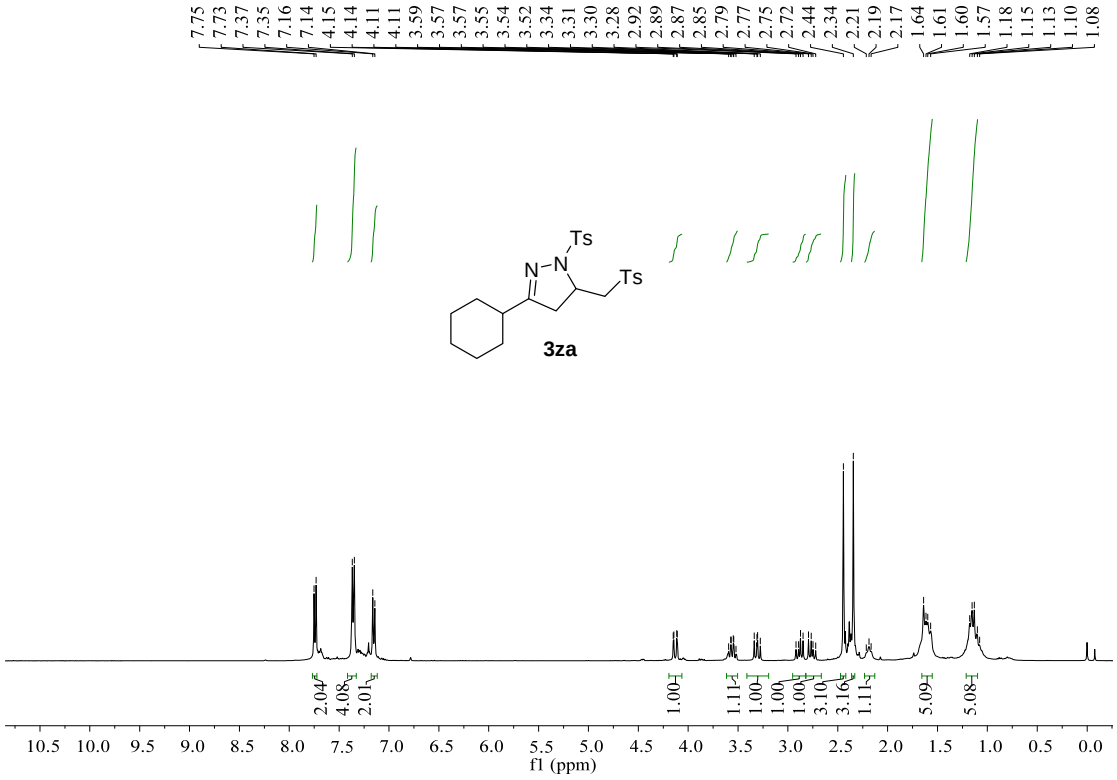
60.70
56.93
40.80
21.81
21.70
Ts
N
N
Ts
S
3ya
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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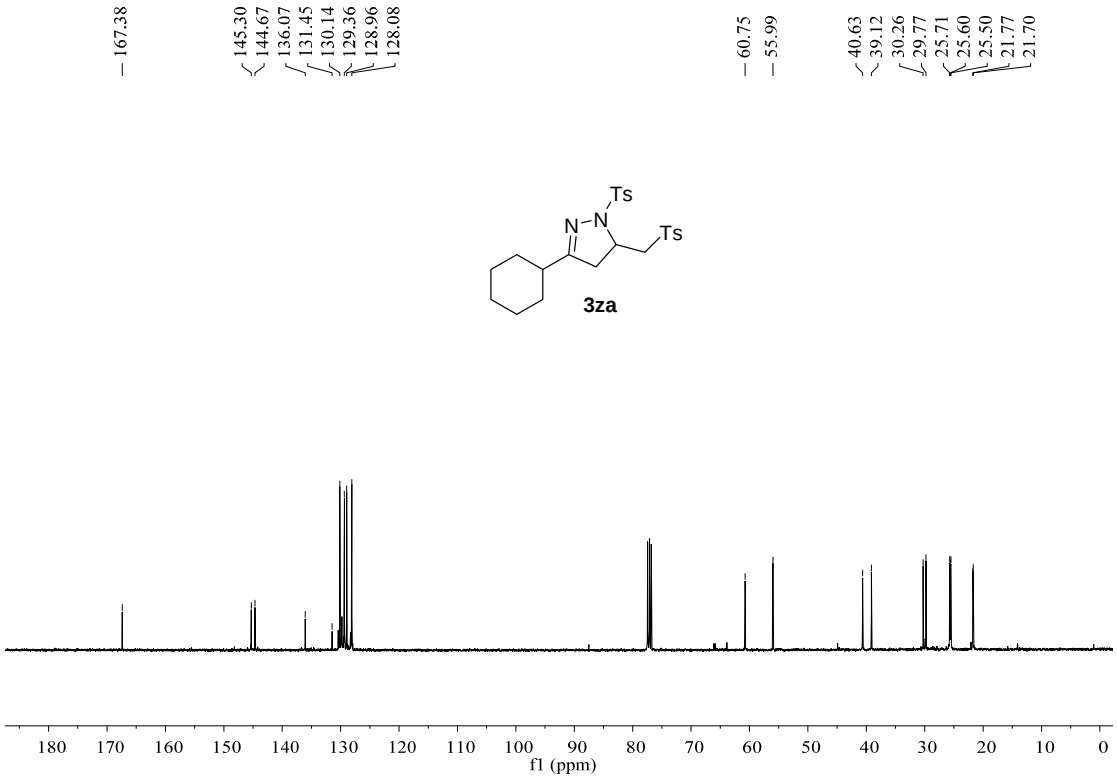
7.37
7.35
7.16
7.14
4.15
4.14
4.11
4.11
3.59
3.57
3.57
3.55
3.54
3.52
3.34
3.31
3.30
3.28
2.92
2.89
2.87
2.85
2.79
2.77
2.75
2.72
2.44
2.34
2.21
2.19
2.17
1.64
1.61
1.60
1.57
1.18
1.15
1.13
1.10
1.08
Ts
N
N
Ts
3za
2.04
4.08
2.01
1.00
1.11
1.00
1.00
1.00
3.10
3.16
1.11
5.09
5.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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144.67
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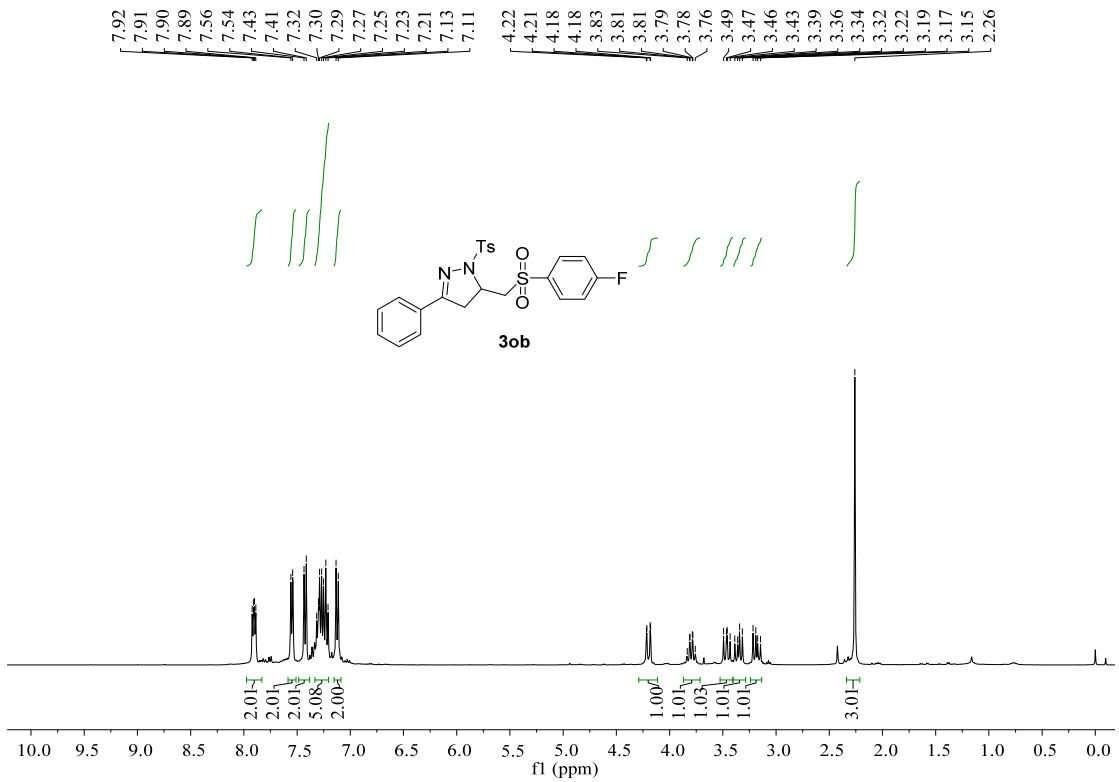
131.45
130.14
129.36
128.96
128.08
60.75
55.99
40.63
39.12
30.26
29.77
25.71
25.60
25.50
21.77
21.70
Ts
N
N
Ts
3za
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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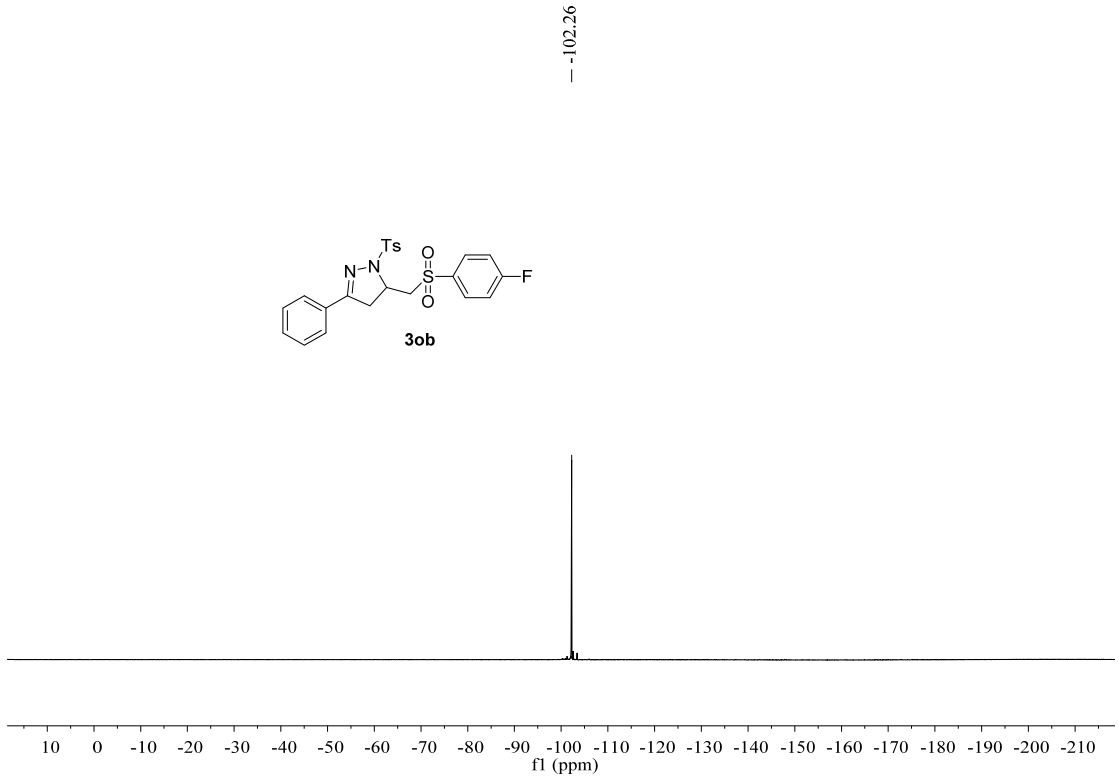
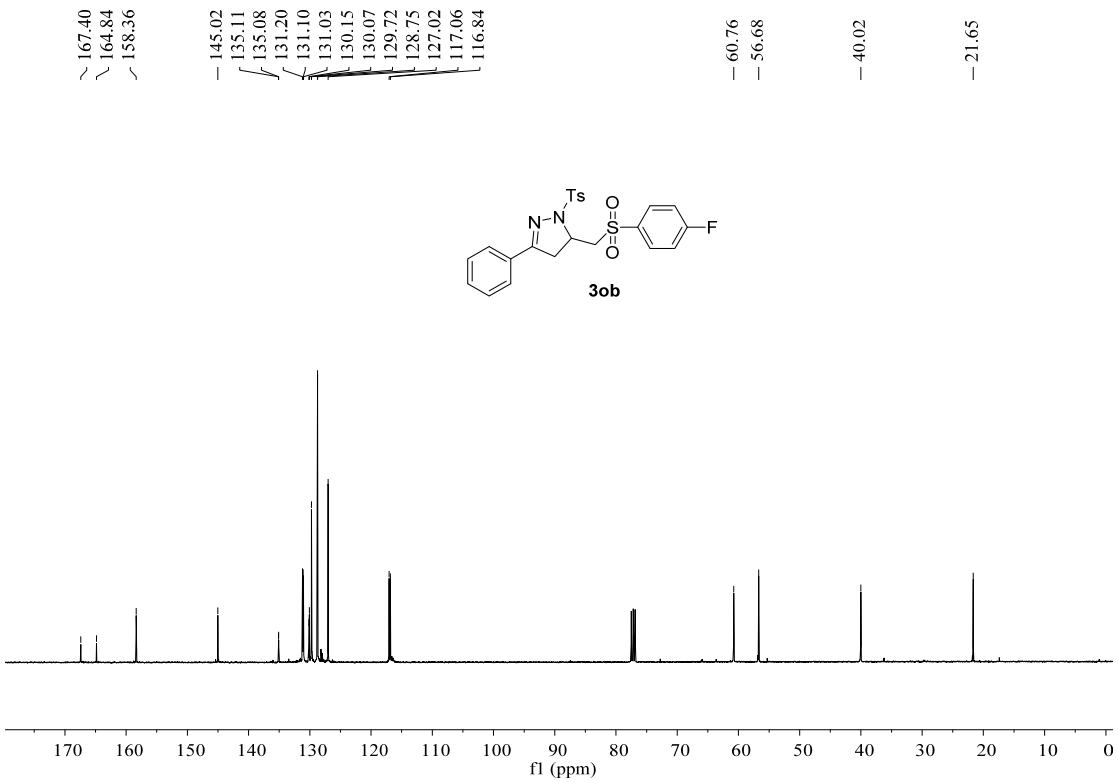
7.54
7.43
7.41
7.32
7.30
7.29
7.27
7.25
7.23
7.21
7.13
7.11
4.22
4.21
4.18
4.18
3.83
3.81
3.81
3.79
3.78
3.76
3.49
3.47
3.46
3.43
3.39
3.36
3.34
3.32
3.22
3.19
3.17
3.15
2.26
Ts
N
N
O
S
O
F
3ob
2.01
2.01
2.01
5.08
2.00
1.00
1.01
1.03
1.01
1.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-102.26
Ts
N
N
O
S
O
F
3ob
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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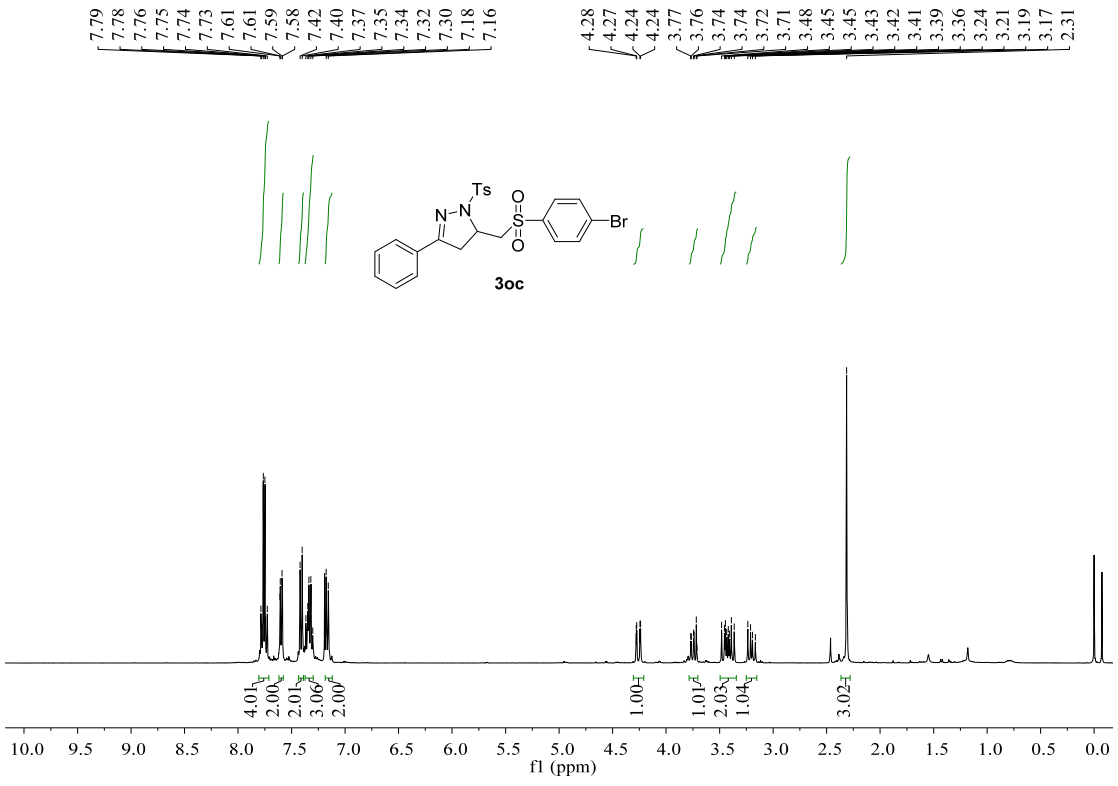
164.84
158.36
145.02
135.11
135.08
131.20
131.10
131.03
130.15
130.07
129.72
128.75
127.02
117.06
116.84
60.76
56.68
40.02
21.65
Ts
N
N
O
S
O
F
3ob
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.61
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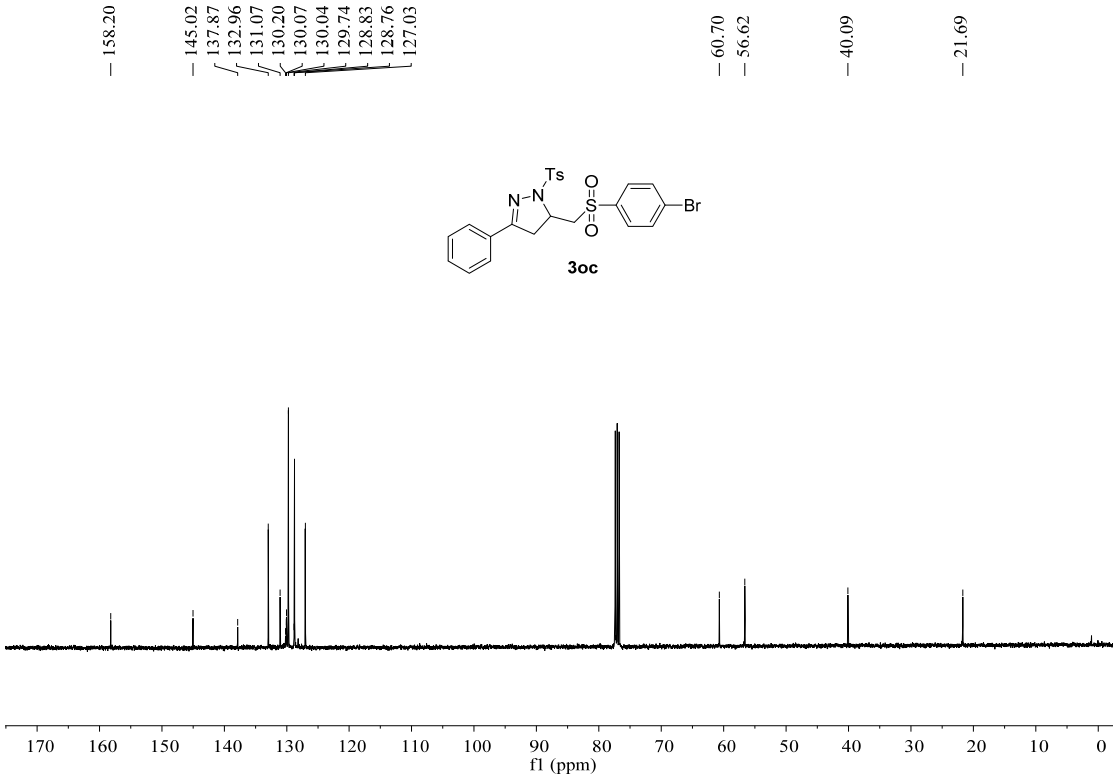
7.58
7.42
7.40
7.37
7.35
7.34
7.32
7.30
7.18
7.16
4.28
4.27
4.24
4.24
3.77
3.76
3.74
3.74
3.72
3.71
3.48
3.45
3.45
3.43
3.42
3.41
3.39
3.36
3.24
3.21
3.19
3.17
2.31
Ts
N
N
O
S
O
Br
3oc
4.01
2.00
2.01
3.06
2.00
1.00
1.01
2.03
1.04
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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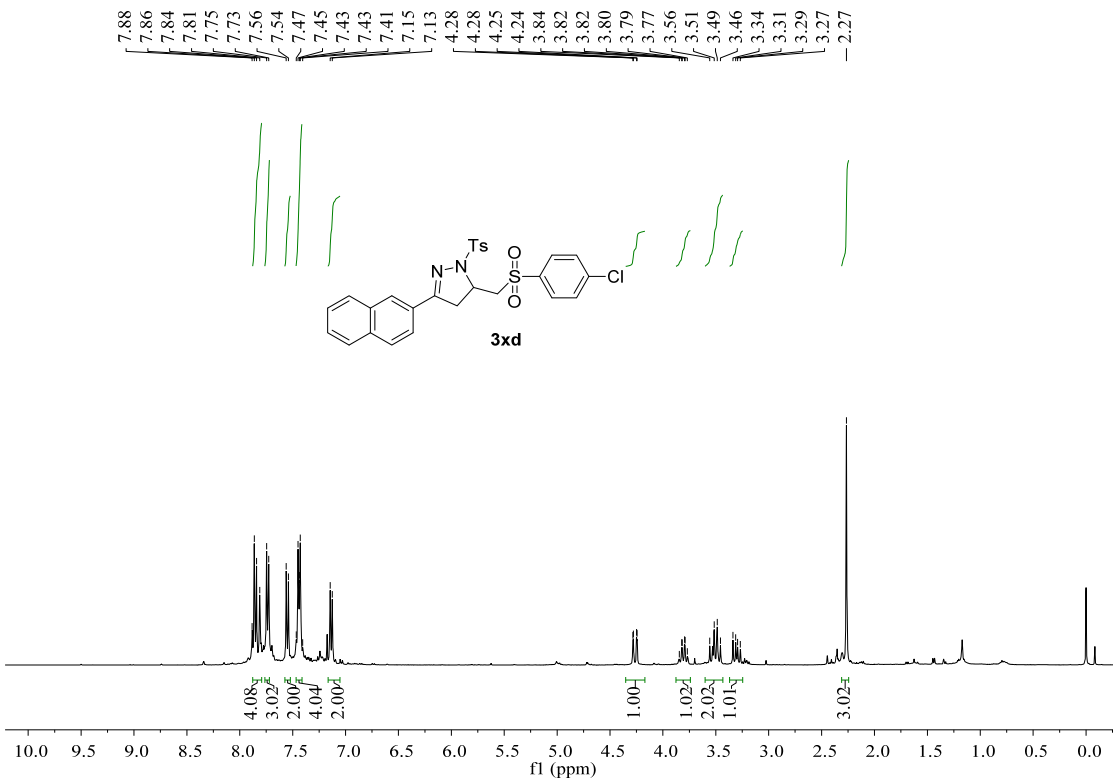
131.07
130.20
130.07
130.04
129.74
128.83
128.76
127.03
60.70
56.62
40.09
21.69
Ts
N
N
O
S
O
Br
3oc
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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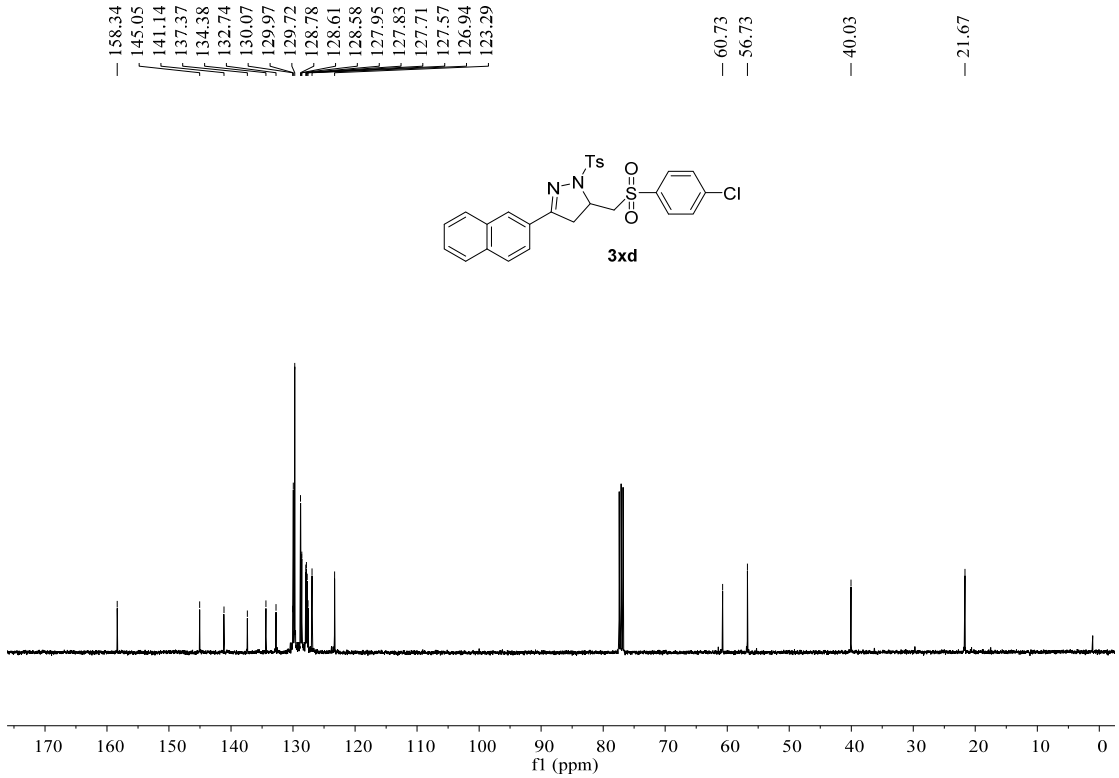
7.43
7.41
7.15
7.13
4.28
4.28
4.25
4.24
3.84
3.82
3.82
3.80
3.79
3.77
3.56
3.51
3.49
3.46
3.34
3.31
3.29
3.27
2.27
Ts
N
N
O
S
O
Cl
3xd
4.08
3.02
2.00
4.04
2.00
1.00
1.02
2.02
1.01
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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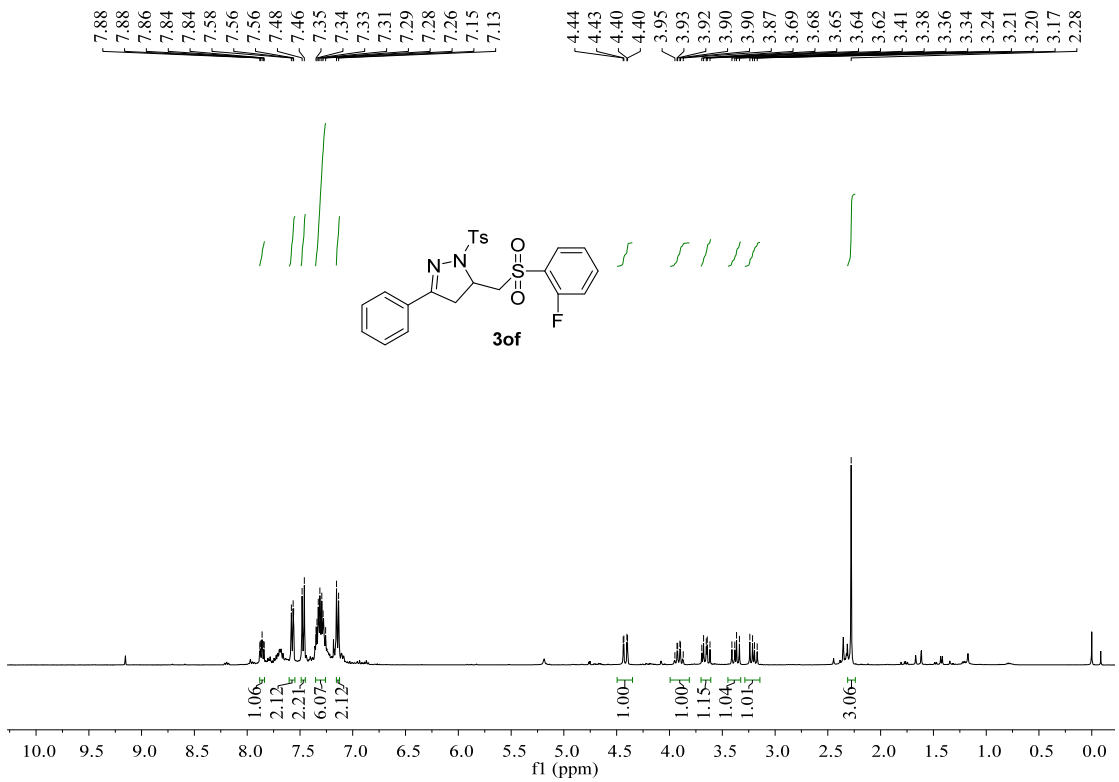
129.97
129.72
128.78
128.61
128.58
127.95
127.83
127.71
127.57
126.94
123.29
60.73
56.73
40.03
21.67
Ts
N
N
O
S
O
Cl
3xd
f1 (ppm)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7.84
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7.56
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7.46
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7.33
7.31
7.29
7.28
7.26
7.15
7.13
4.44
4.43
4.40
4.40
3.95
3.93
3.92
3.90
3.90
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3.68
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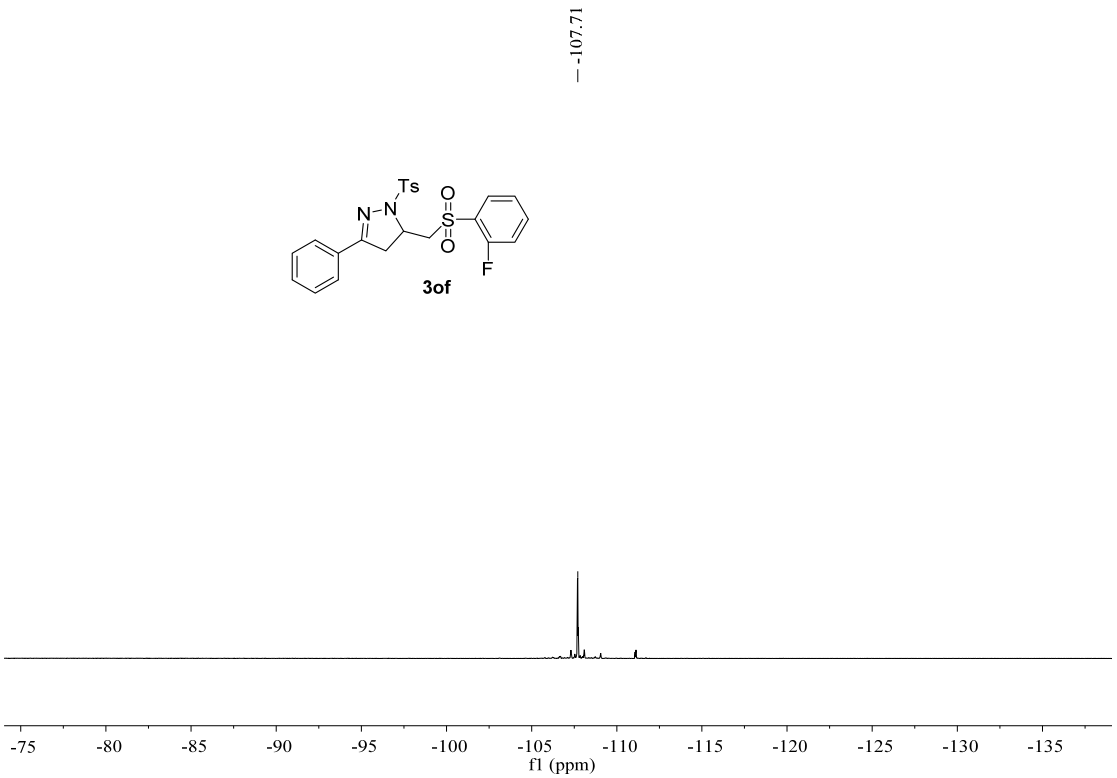
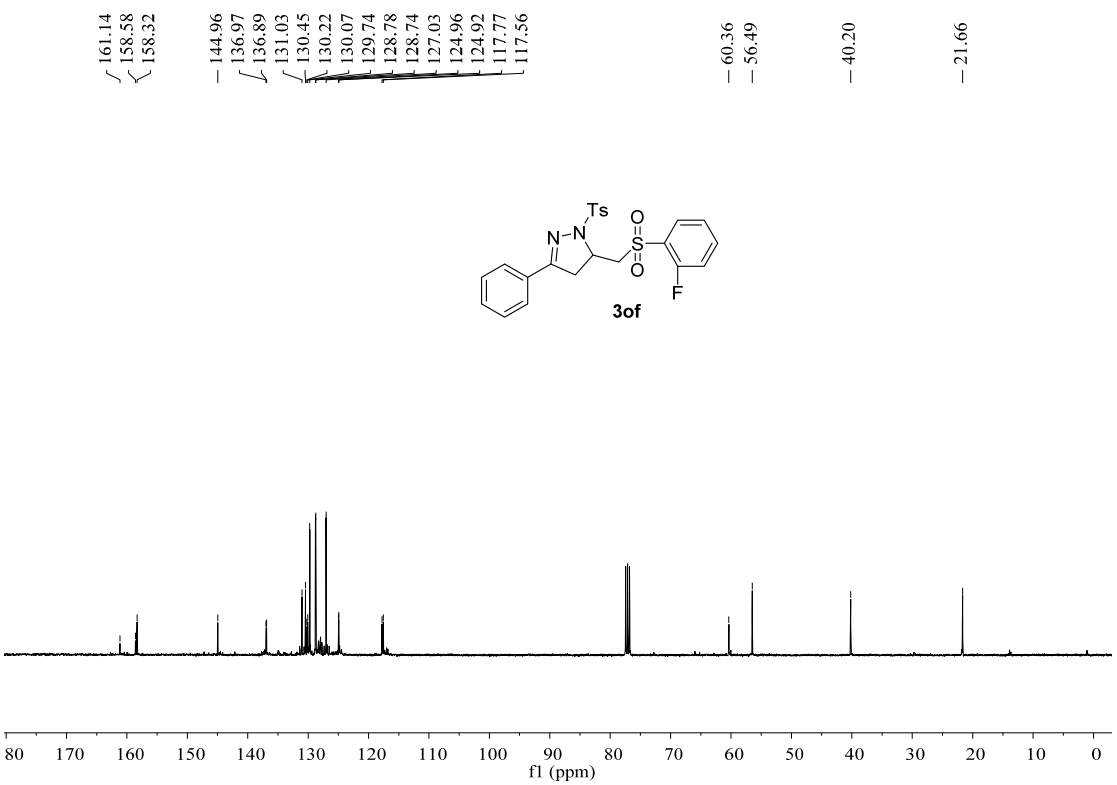
3.62
3.41
3.38
3.36
3.34
3.24
3.21
3.20
3.17
2.28
Ts
N
N
O
S
O
F
3of
1.06
2.12
2.21
6.07
2.12
1.00
1.00
1.15
1.04
1.01
3.06
f1 (ppm)


-107.71
Ts
N
N
O
S
O
F
3of
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
f1 (ppm)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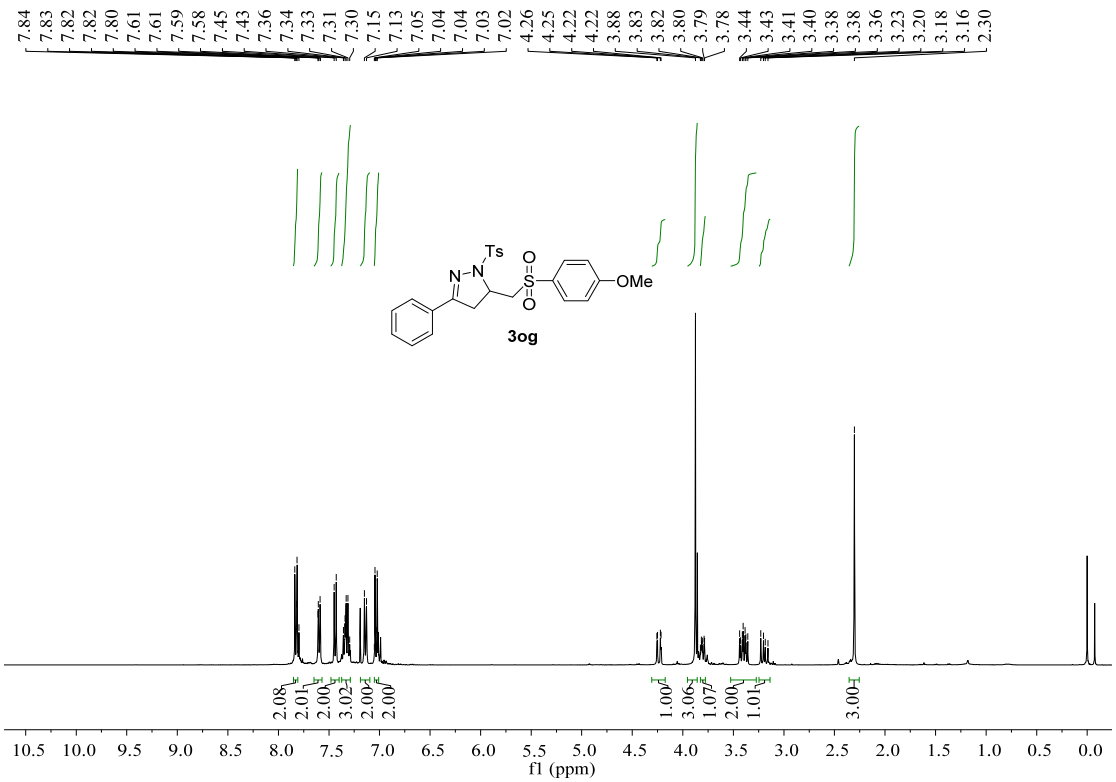
131.03
130.45
130.22
130.07
129.74
128.78
128.74
127.03
124.96
124.92
117.77
117.56
60.36
56.49
40.20
21.66
Ts
N
N
O
S
O
F
3of
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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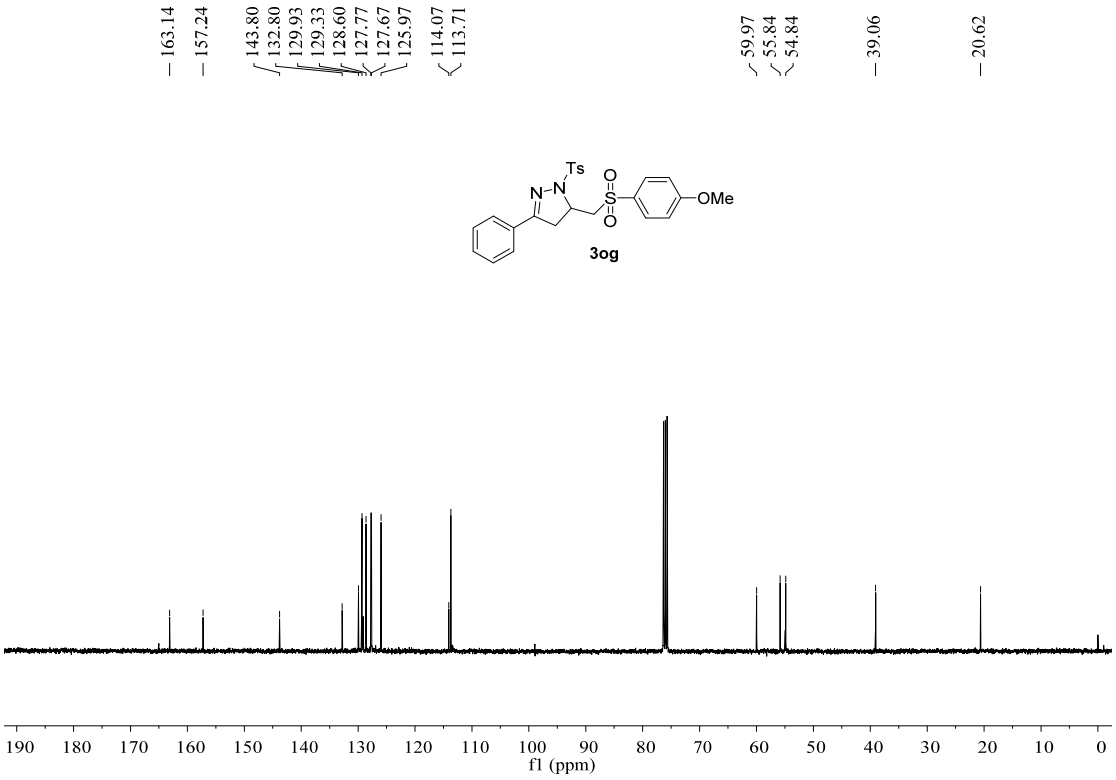
7.61
7.59
7.58
7.45
7.43
7.36
7.34
7.33
7.31
7.30
7.15
7.13
7.05
7.04
7.04
7.03
7.02
4.26
4.25
4.22
4.22
3.88
3.83
3.82
3.80
3.79
3.78
3.44
3.43
3.41
3.40
3.38
3.38
3.36
3.23
3.20
3.18
3.16
2.30
Ts
N
N
O
S
O
OMe
3og
2.08
2.01
2.00
3.02
2.00
2.00
1.00
3.06
1.07
2.00
1.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.67
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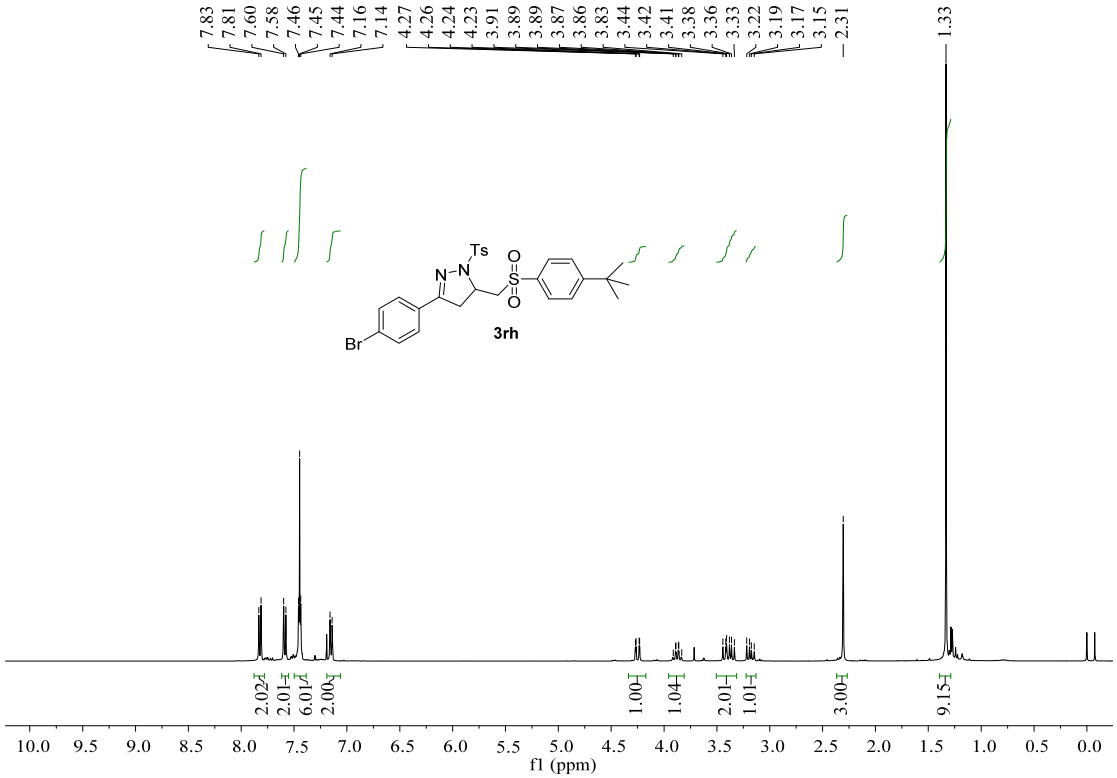
114.07
113.71
59.97
55.84
54.84
39.06
20.62
Ts
N
N
O
S
O
OMe
3og
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.81
7.60
7.58
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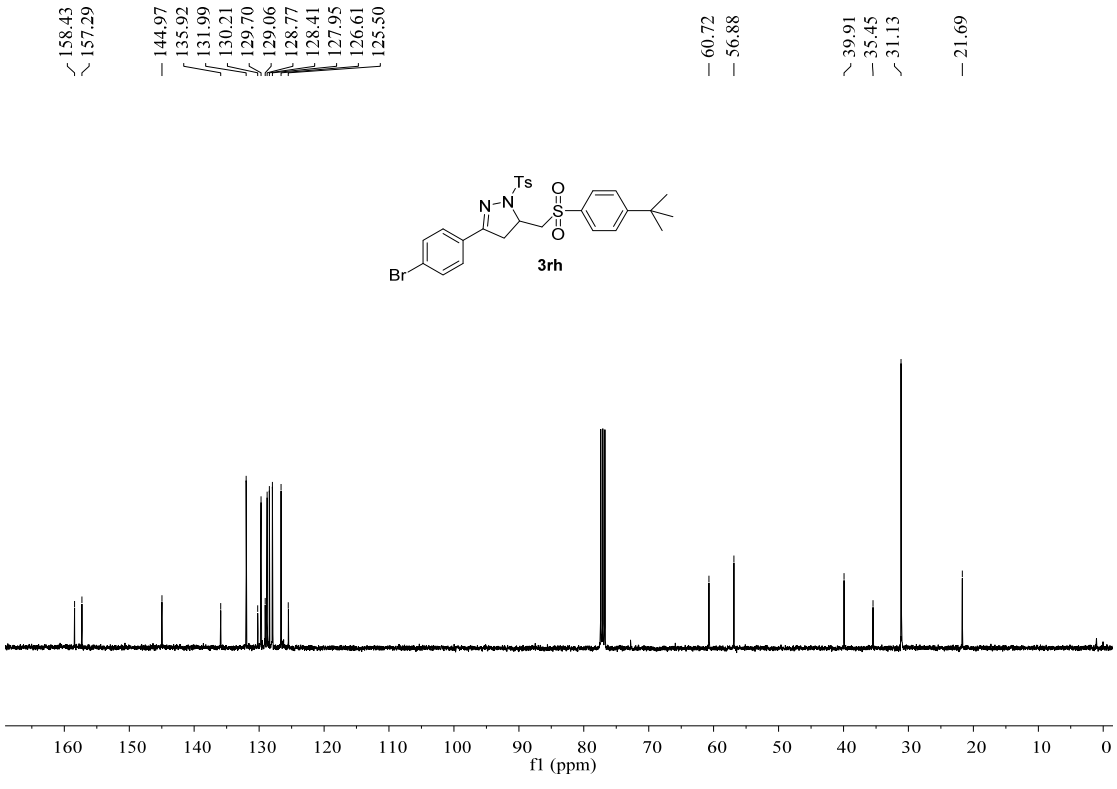
7.45
7.44
7.16
7.14
4.27
4.26
4.24
4.23
3.91
3.89
3.89
3.87
3.86
3.83
3.44
3.42
3.41
3.38
3.36
3.33
3.22
3.19
3.17
3.15
2.31
1.33
Ts
N
N
O
S
O
Br
3rh
2.02
2.01
6.01
2.00
1.00
1.04
2.01
1.01
3.00
9.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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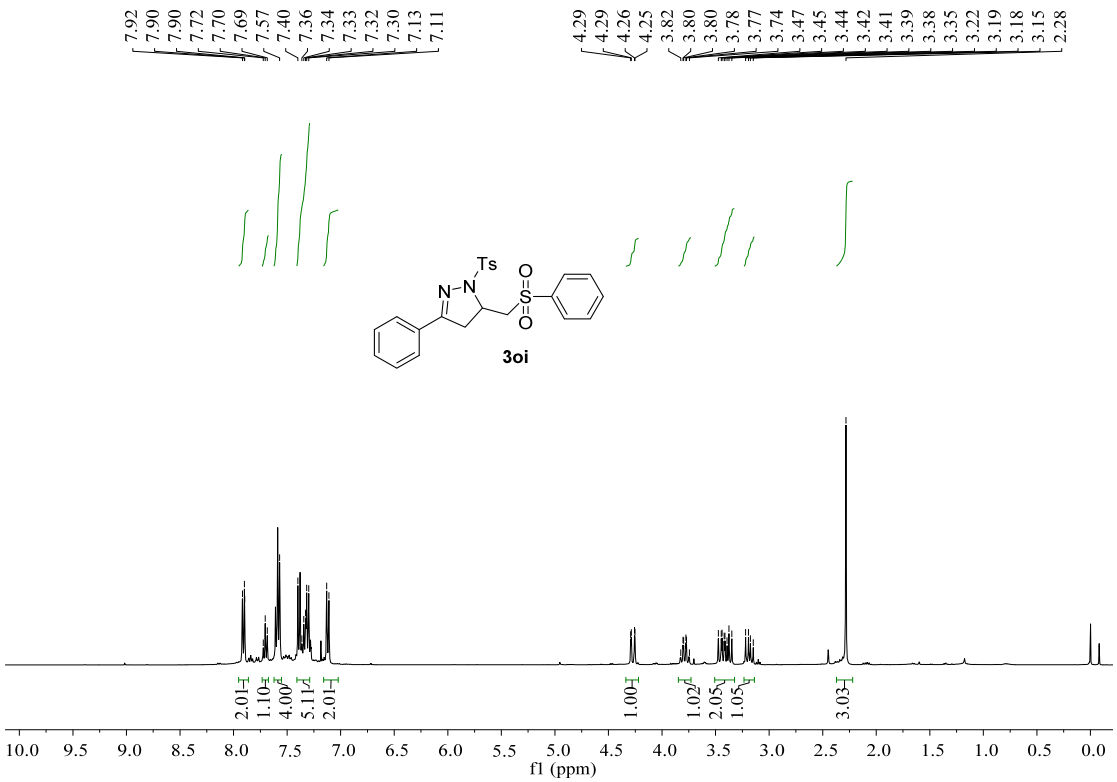
157.29
144.97
135.92
131.99
130.21
129.70
129.06
128.77
128.41
127.95
126.61
125.50
60.72
56.88
39.91
35.45
31.13
21.69
Ts
N
N
O
S
O
Br
3rh
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.90
7.90
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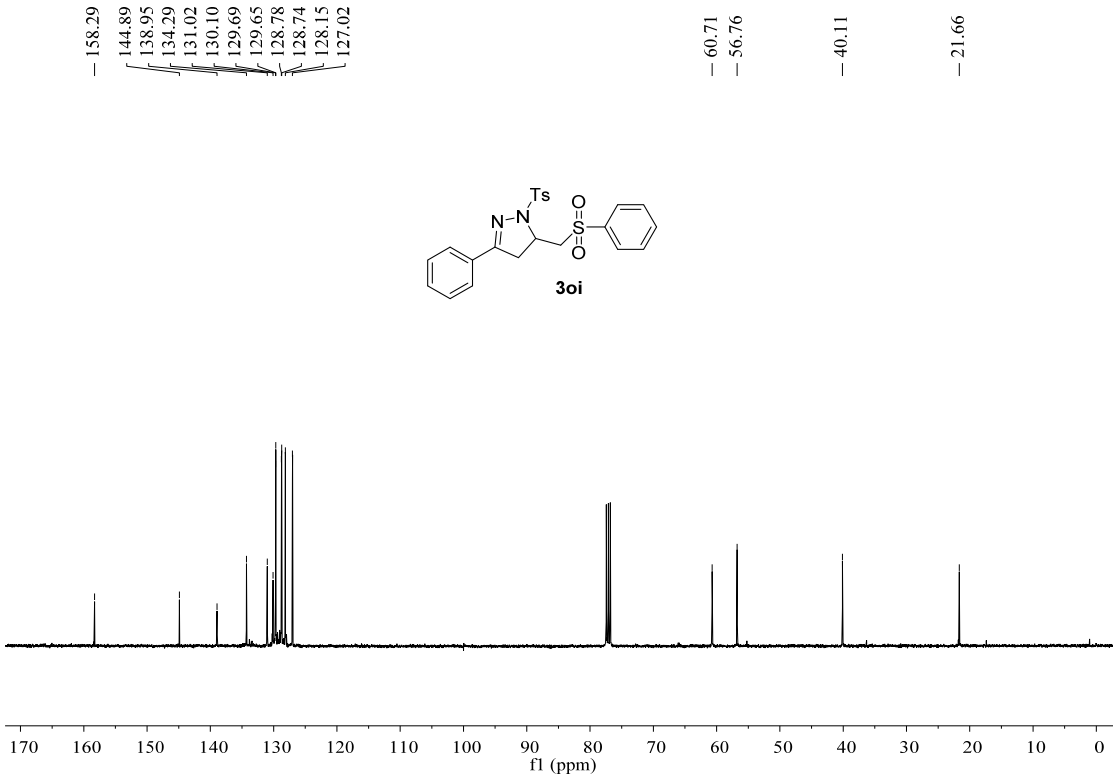
7.69
7.57
7.40
7.36
7.34
7.33
7.32
7.30
7.13
7.11
4.29
4.29
4.26
4.25
3.82
3.80
3.80
3.78
3.77
3.74
3.47
3.45
3.44
3.42
3.41
3.39
3.38
3.35
3.22
3.19
3.18
3.15
2.28
Ts
N
N
O
S
O
3oi
2.01
1.10
4.00
5.11
2.01
1.00
1.02
2.05
1.05
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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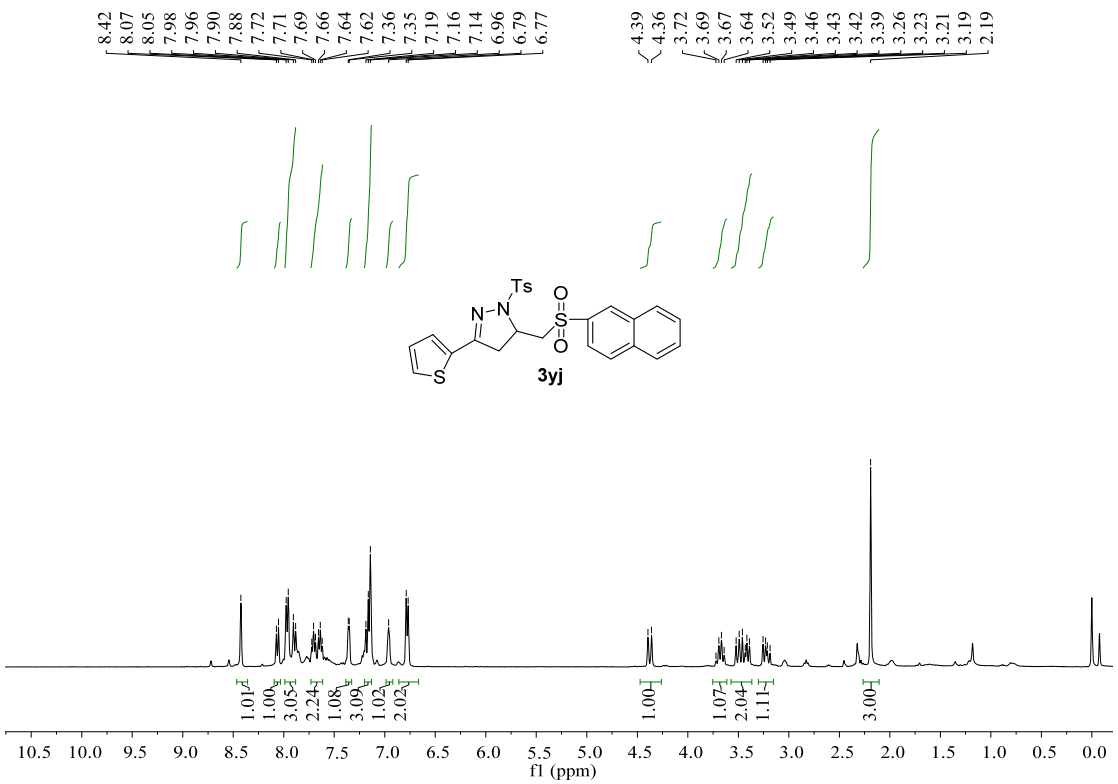
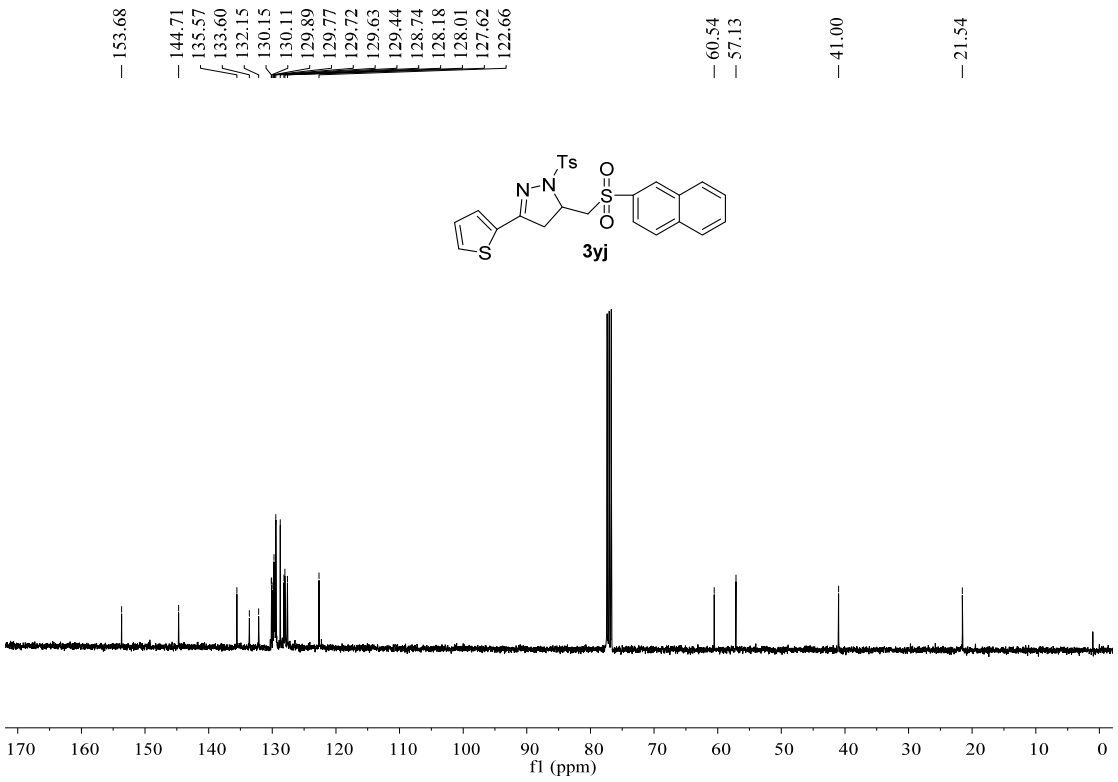
144.89
138.95
134.29
131.02
130.10
129.69
129.65
128.78
128.74
128.15
127.02
60.71
56.76
40.11
21.66
Ts
N
N
O
S
O
3oi
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.42
8.07
8.05
7.98
7.96
7.90
7.88
7.72
7.71
7.69
7.66
7.64
7.62
7.36
7.35
7.19
7.16
7.14
6.96
6.79
6.77
4.39
4.36
3.72
3.69
3.67
3.64
3.52
3.49
3.46
3.43
3.42
3.39
3.26
3.23
3.21
3.19
2.19
Ts
N
N
O
S
O
S
3yj
1.01
1.00
3.05
2.24
1.08
3.09
1.02
2.02
1.00
1.07
2.04
1.11
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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144.71
135.57
133.60
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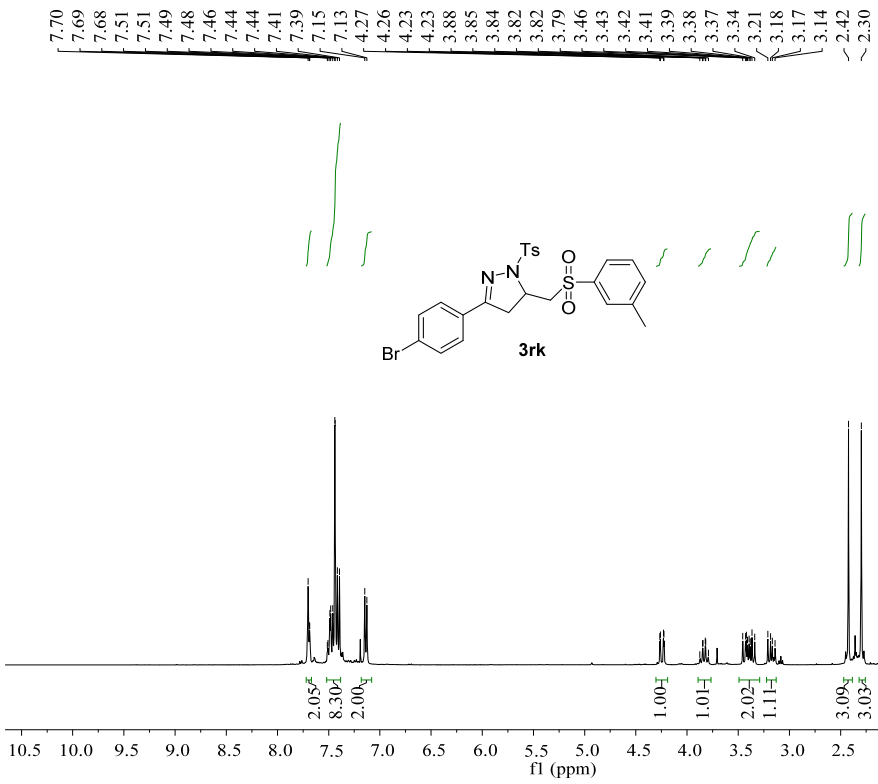
130.15
130.11
129.89
129.77
129.72
129.63
129.44
128.74
128.18
128.01
127.62
122.66
60.54
57.13
41.00
21.54
Ts
N
N
O
S
O
S
3yj
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.69
7.68
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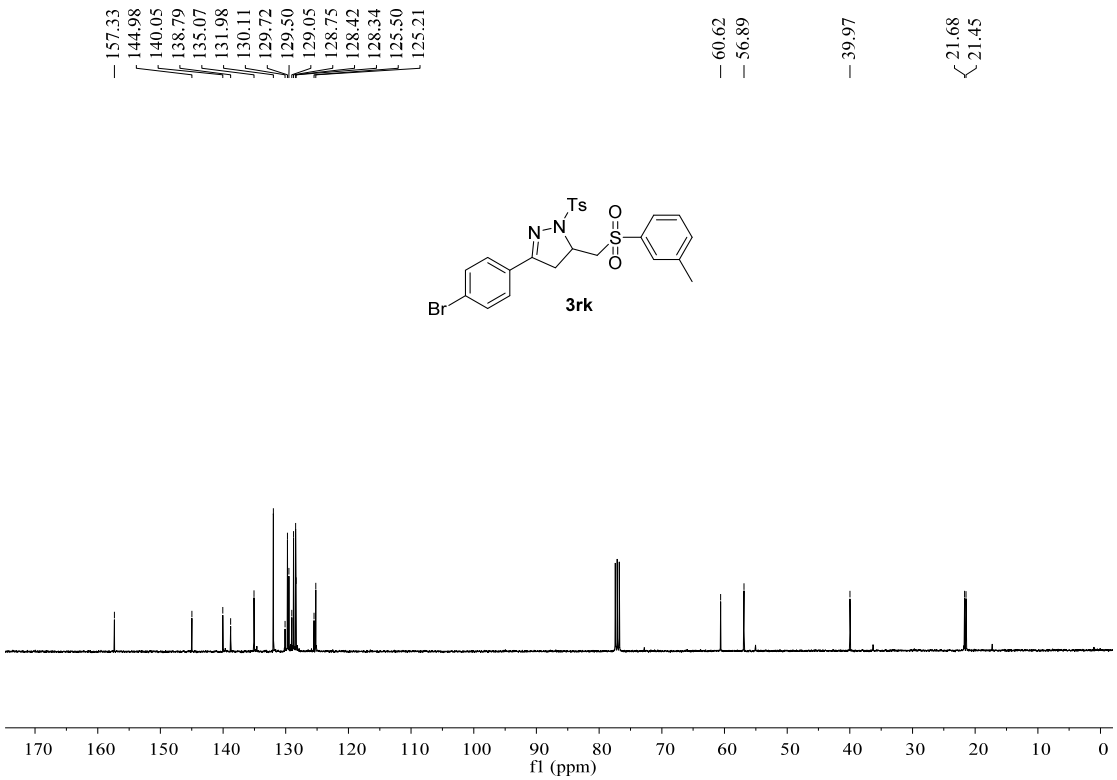
7.51
7.49
7.48
7.46
7.44
7.44
7.41
7.39
7.15
7.13
4.27
4.26
4.23
4.23
3.88
3.85
3.84
3.82
3.82
3.79
3.46
3.43
3.42
3.41
3.39
3.38
3.37
3.34
3.21
3.18
3.17
3.14
2.42
2.30
Ts
N
N
O
S
O
Br
3rk
2.05
8.30
2.00
1.00
1.01
2.02
1.11
3.09
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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140.05
138.79
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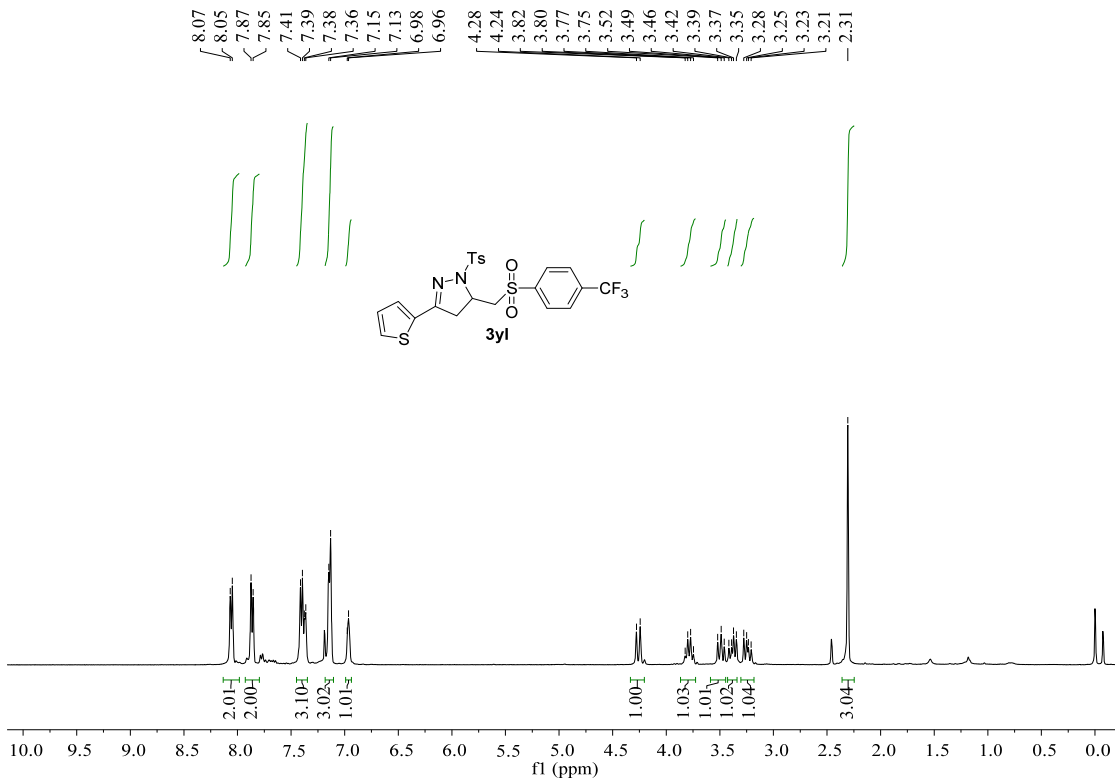
131.98
130.11
129.72
129.50
129.05
128.75
128.42
128.34
125.50
125.21
60.62
56.89
39.97
21.68
21.45
Ts
N
N
O
S
O
Br
3rk
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.07
8.05
7.87
7.85
7.41
7.39
7.38
7.36
7.15
7.13
6.98
6.96
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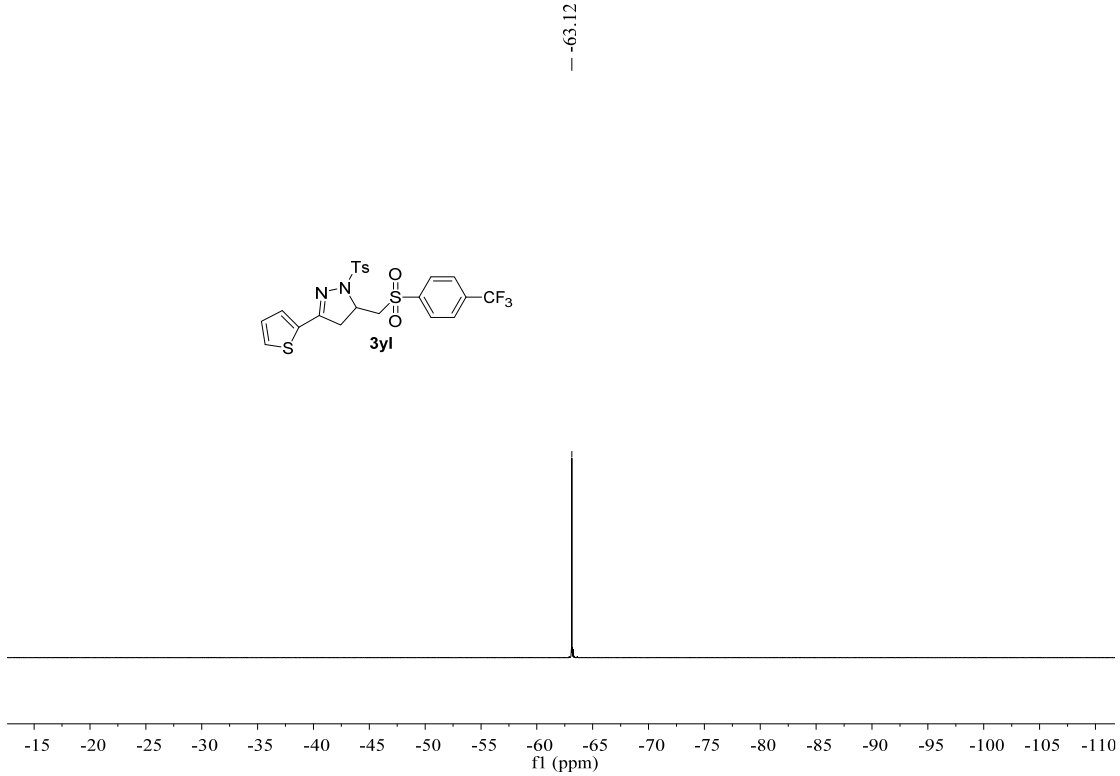
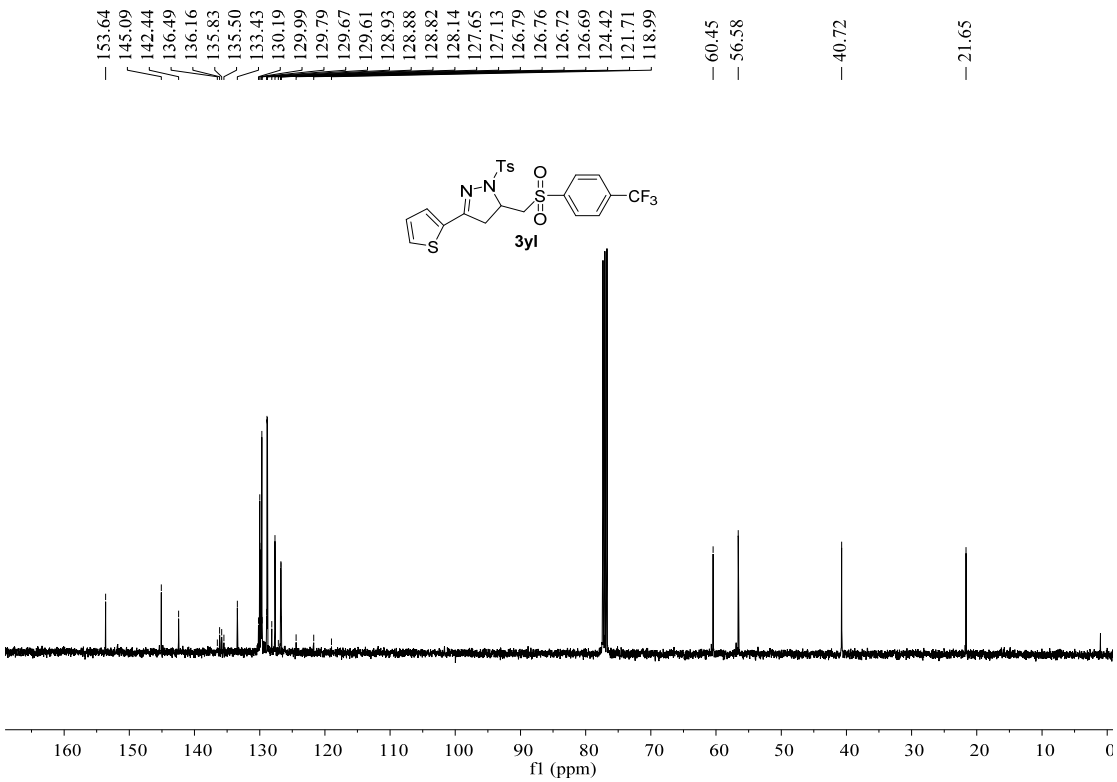
4.24
3.82
3.80
3.77
3.75
3.52
3.49
3.46
3.42
3.39
3.37
3.35
3.28
3.25
3.23
3.21
2.31
Ts
N
N
O
S
O
CF3
S
3yl
2.01
2.00
3.10
3.02
1.01
1.00
1.03
1.01
1.02
1.04
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-63.12
Ts
N
N
O
S
O
CF3
S
3yl
-15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110
f1 (ppm)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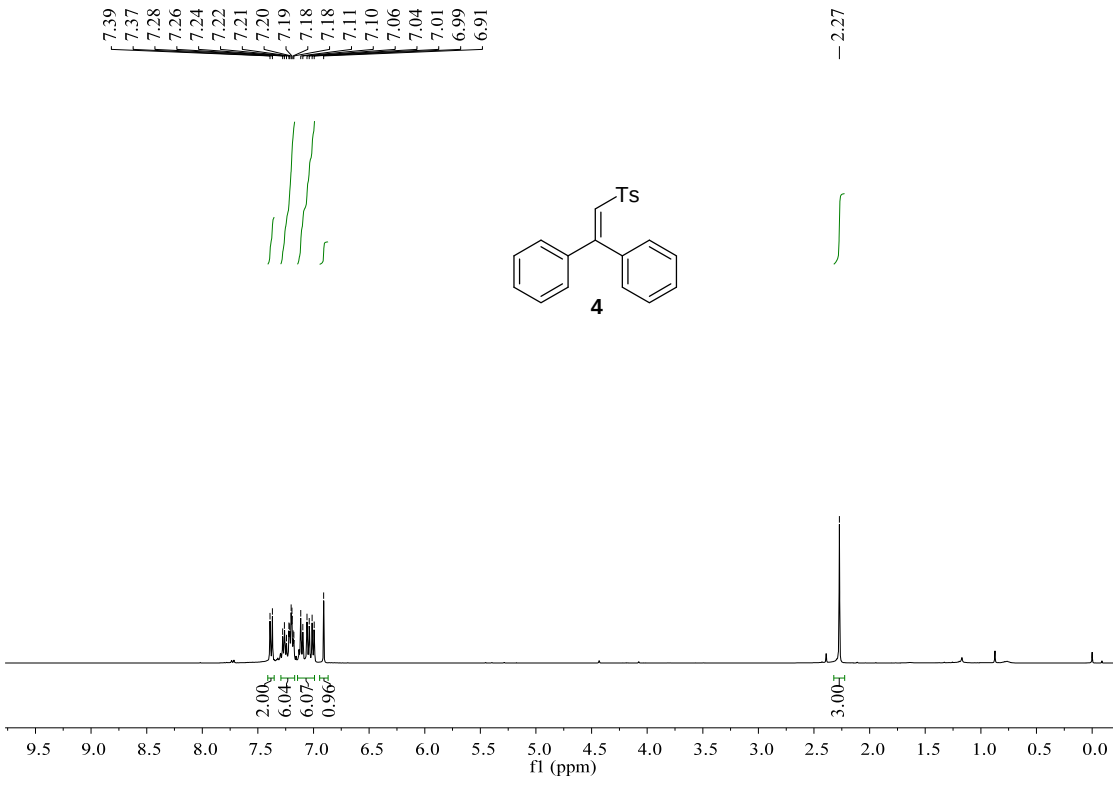
135.50
133.43
130.19
129.99
129.79
129.67
129.61
128.93
128.88
128.82
128.14
127.65
127.13
126.79
126.76
126.72
126.69
124.42
121.71
118.99
60.45
56.58
40.72
21.65
Ts
N
N
O
S
O
CF3
S
3yl
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.37
7.28
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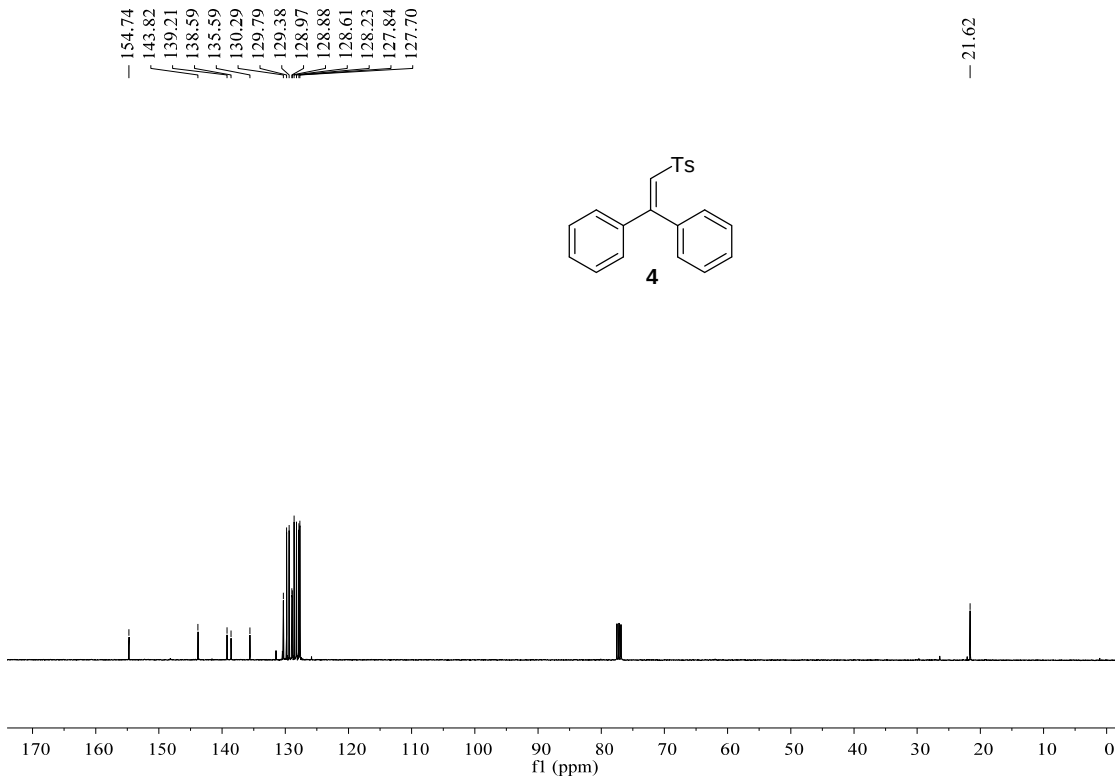
7.24
7.22
7.21
7.20
7.19
7.18
7.18
7.11
7.10
7.06
7.04
7.01
6.99
6.91
2.27
Ts
4
2.00
6.04
6.07
0.96
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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143.82
139.21
138.59
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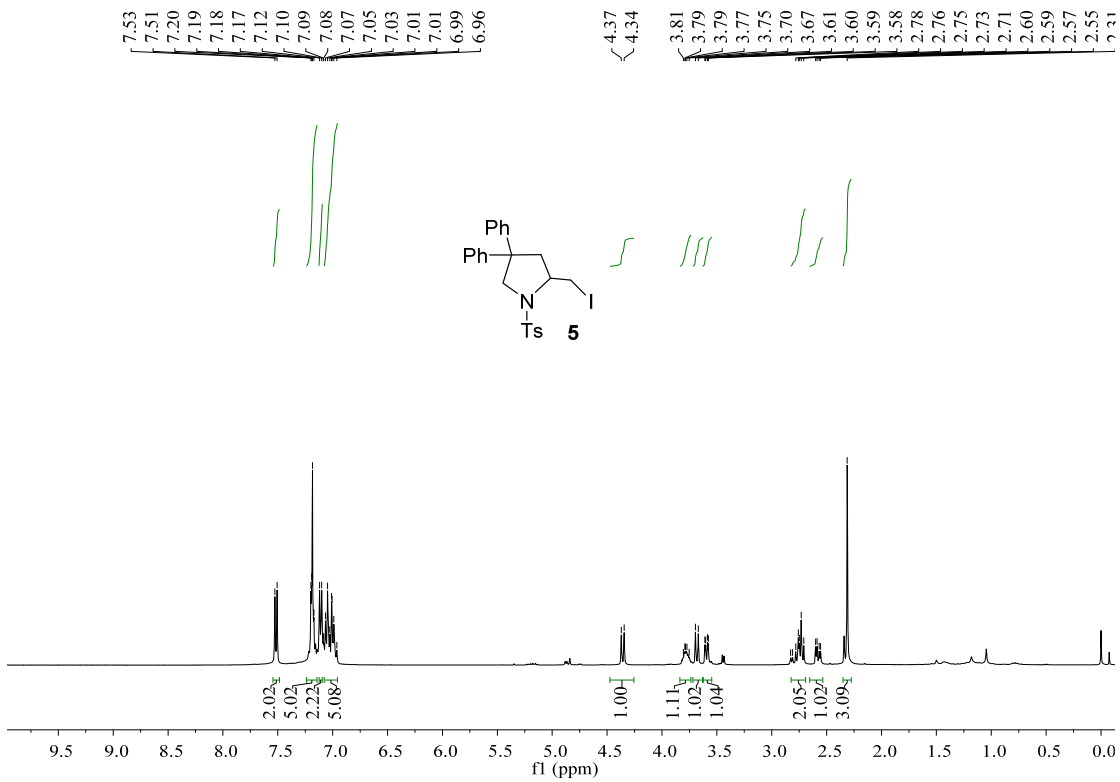
130.29
129.79
129.38
128.97
128.88
128.61
128.23
127.84
127.70
21.62
Ts
4
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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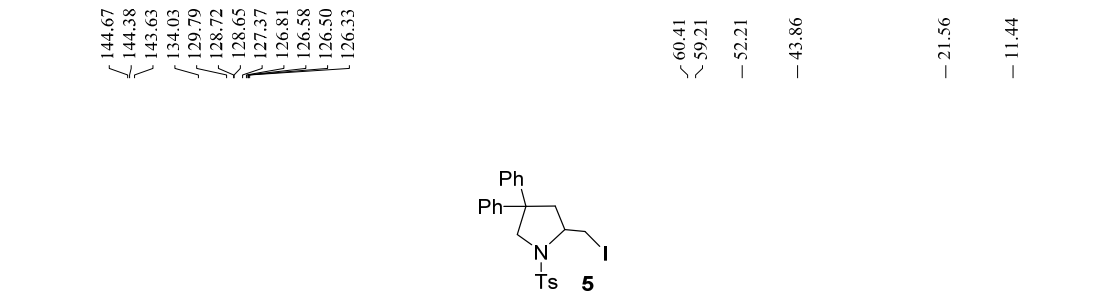
7.17
7.12
7.10
7.09
7.08
7.07
7.05
7.03
7.01
7.01
6.99
6.96
4.37
4.34
3.81
3.79
3.79
3.77
3.75
3.70
3.67
3.61
3.60
3.59
3.58
2.78
2.76
2.75
2.73
2.71
2.60
2.59
2.57
2.55
Ph
Ph
N
Ts
I
5
2.02
5.02
2.22
5.08
1.00
1.11
1.02
1.04
2.05
1.02
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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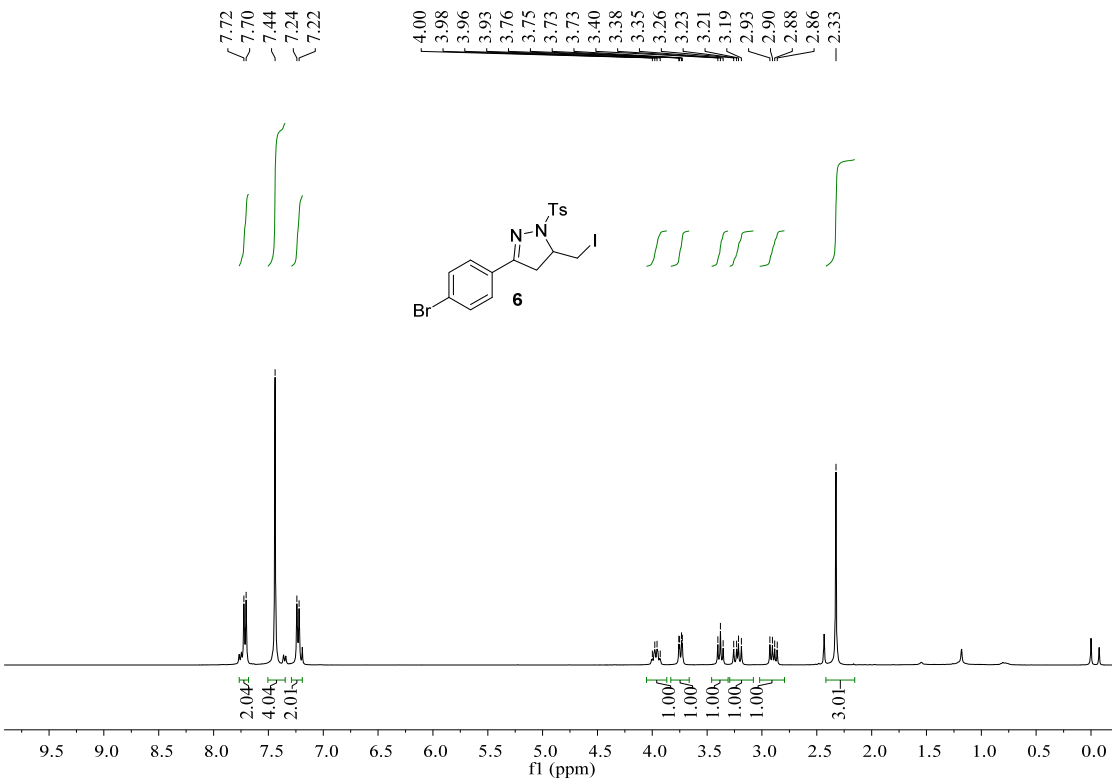
128.72
128.65
127.37
126.81
126.58
126.50
126.33
60.41
59.21
52.21
43.86
21.56
11.44
Ph
Ph
N
Ts
I
5
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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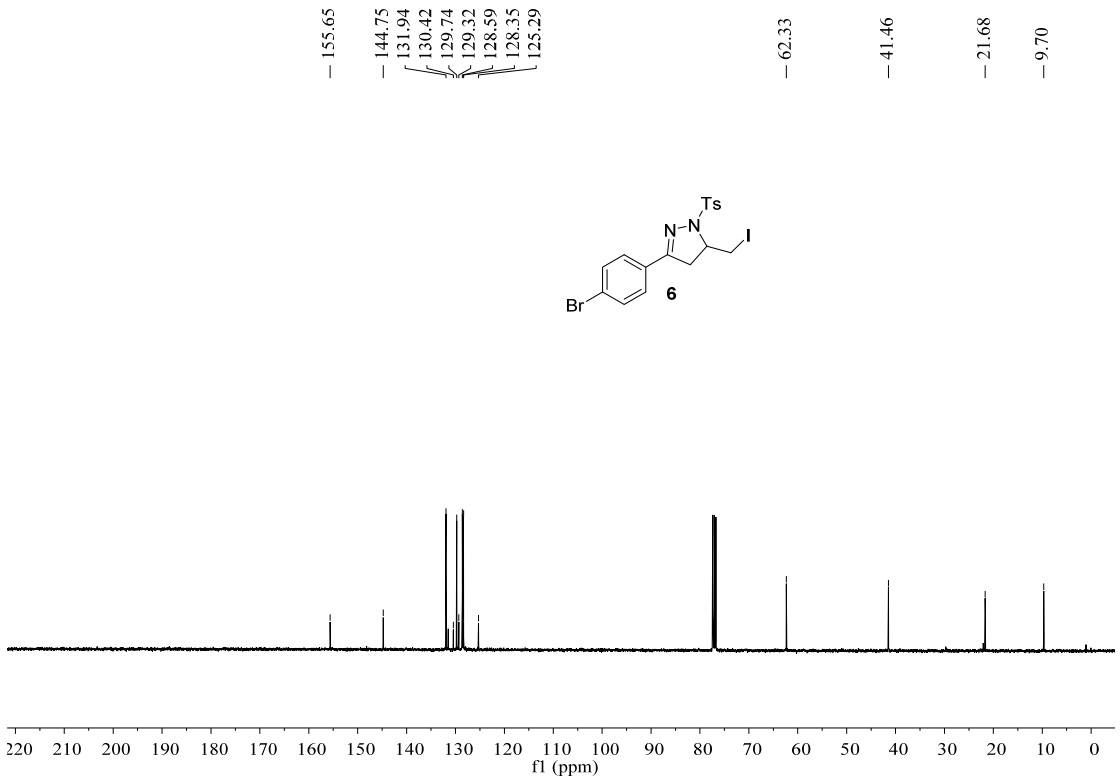
7.22
4.00
3.98
3.96
3.93
3.76
3.75
3.73
3.73
3.40
3.38
3.35
3.26
3.23
3.21
3.19
2.93
2.90
2.88
2.86
2.33
Ts
N
N
I
Br
6
2.04
4.04
2.01
1.00
1.00
1.00
1.00
1.00
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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144.75
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130.42
129.74
129.32
128.59
128.35
125.29
62.33
41.46
21.68
9.70
Ts
N
N
I
Br
6
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)