Supporting Information

Synthesis of Trifluoromethylated Pyrazolidines by [3+2] Cycloaddition

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1 General information

Flash chromatography was performed using silica gel 60 (230-400 mesh). Analytical thin layer chromatography (TLC) was done using silica Gel (silica gel GF254). TLC plates were analysed by an exposure to ultraviolet (UV) light and/or in iodine vapour. High-resolution mass spectra were recorded on Fourier transform ion cyclotron resonance mass spectrometer. NMR experiments were carried out in deuterochloroform ($CDCl_3$) or deuterated acetone ($(CD_3)_2CO$). ^1H NMR, ^{13}C NMR spectra were recorded at 400 MHz or 600 MHz and 100 MHz or 150 MHz spectrometers, respectively. ^{19}F NMR spectra were recorded at 376 MHz spectrometers. Chemical shifts are reported as δ values relative to internal TMS (δ 0.00 for ^1H NMR), chloroform (δ 7.26 for ^1H NMR), acetone (δ 2.05 for ^1H NMR), chloroform (δ 77.00 for ^{13}C NMR), acetone (δ 206.26 for ^{13}C NMR) in parts per million (ppm). The following abbreviations are used for the multiplicities: s: singlet, d: doublet, dd: doublet of doublet, t: triplet, td: doublet of triplet, q: quadruplet, m: multiplet, br: broad signal for proton spectra; Coupling constants (*J*) are reported in Hertz (Hz). Melting points were uncorrected. The solvents were distilled by standard methods. Reagents were obtained from commercial suppliers and used without further purification unless otherwise noted.

2 General procedure for [3+2] cycloaddition reaction

A solution of trifluoromethylated *N*-acylhyrazones **1** (0.2 mmol), nitroolefins **2** (0.7 mmol), KOH (0.3 mmol) and Bu_4NI (0.02 mmol) in CH_3CN (5 mL) was stirred at room temperature for 6-24 h and monitored by thin layer chromatography (TLC) until the starting materials were not detected. CH_3CN was removed from the reaction mixture under vacuum. The saturated NH_4Cl solution (10 mL) was poured into the mixture and stirred for 10 min, then the mixture was extracted with EtOAc (3 × 10 mL). The combined organic extracts were dried ($MgSO_4$) and concentrated. Purification of the residue by silica gel column chromatography using petroleum ether : acetone (4 : 1) as eluent furnished the products **3**.

3 General experimental procedures for the synthesis of compounds 4

A solution of trifluoromethylated pyrazolidine **3** (0.1 mmol), 3.0 equiv. of $CuCl_2$ in EtOH (4 mL) was stirred at reflux for 6-8 h and monitored by thin layer chromatography (TLC) until the starting material was not detected, the reaction mixture was cooled to room temperature. The solid was filtrated from the reaction mixture. The filtrate was concentrated in vacuum. Purification of the residue by silica gel column chromatography using petroleum ether : acetone (4 : 1) as eluent furnished the products **4**.

4 X-ray Diffraction Structure of 3aa

Figure S1. Diffraction Structure of 3aa; thermal ellipsoids are set at a 50% probability level

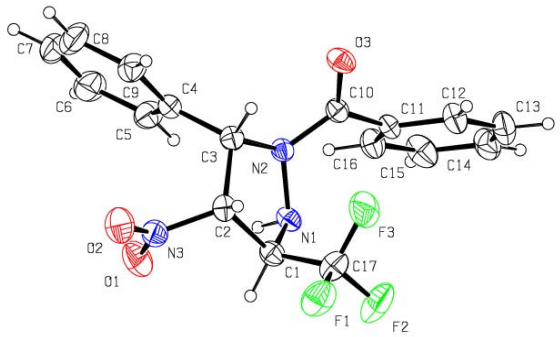


Table S1 Crystal data and structure refinement for 3aa.

Identification code	PXS_1
Empirical formula	$C_{17}H_{14}F_3N_3O_3$
Formula weight	365.31
Temperature/K	292.76(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.6912(4)
b/Å	25.2938(19)
c/Å	11.9374(9)
α/°	90
β/°	102.064(8)
γ/°	90
Volume/Å^3	1680.5(2)
Z	4
ρ_{calc}g/cm^3	1.444
μ/mm^{-1}	0.123
F(000)	752.0
Crystal size/mm^3	0.22 × 0.17 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.98 to 52.044
Index ranges	-5 ≤ h ≤ 7, -24 ≤ k ≤ 31, -13 ≤ l ≤ 14
Reflections collected	6343
Independent reflections	3289 [R_{int} = 0.0422, R_{sigma} = 0.0817]
Data/restraints/parameters	3289/0/239
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0646, wR_2 = 0.1172
Final R indexes [all data]	R_1 = 0.1220, wR_2 = 0.1501
Largest diff. peak/hole / e Å^{-3}	0.18/-0.24

Table S2 Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for PXS_1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	7152(4)	-463.4(7)	7226.8(18)	81.3(7)
F2	8903(5)	-201.4(9)	8895.6(17)	97.3(9)
F3	5571(4)	154.6(9)	8065.8(19)	83.4(7)
O1	11033(5)	705.6(10)	5561(2)	76.5(8)
O2	7883(5)	476.2(11)	4326.6(19)	82.3(9)
O3	4134(4)	1436.7(8)	8084.4(17)	50.4(6)
N1	9644(5)	823.7(10)	8083(2)	40.9(7)
N2	7683(4)	1178.9(9)	7707.1(19)	36.8(6)
N3	8942(6)	579.6(10)	5294(2)	51.6(7)
C1	9052(5)	362.6(11)	7347(2)	43.3(8)
C2	7498(5)	558.3(11)	6208(2)	40.1(7)
C3	6612(5)	1116.6(11)	6480(2)	39.0(7)
C4	7173(5)	1564.0(12)	5747(2)	41.8(8)
C5	9243(6)	1864.4(14)	6043(3)	57.6(9)
C6	9726(7)	2263.9(14)	5330(4)	73.1(12)
C7	8132(9)	2370.6(15)	4330(3)	76.2(12)
C8	6053(8)	2083.7(16)	4035(3)	76.2(13)
C9	5583(6)	1681.4(13)	4740(3)	57.7(10)
C10	6242(5)	1309.6(11)	8449(2)	38.1(7)
C11	7352(5)	1334.2(11)	9694(2)	38.8(7)
C12	6059(6)	1165.1(13)	10482(3)	54.9(9)
C13	6987(7)	1224.0(15)	11644(3)	70.0(11)
C14	9168(7)	1464.0(15)	12017(3)	66.0(11)
C15	10447(6)	1640.9(15)	11237(3)	64.0(11)
C16	9570(5)	1571.6(12)	10075(3)	50.8(9)
C17	7676(7)	-36.1(14)	7904(3)	60.1(10)

Table S3 Anisotropic displacement parameters ($Å^2×10^3$) for 3aa.
The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	111.4(18)	48.0(12)	80.6(15)	-0.6(11)	11.5(14)	-14.5(12)
F2	144(2)	79.2(15)	58.9(14)	25.3(12)	-0.4(15)	-2.8(15)
F3	82.7(16)	75.1(15)	105.4(18)	9.4(12)	49.6(14)	-13.9(13)
O1	63.8(17)	87(2)	89(2)	-7.9(16)	38.9(15)	-12.9(15)
O2	112(2)	97(2)	37.2(13)	-12.3(13)	14.5(15)	12.9(17)
O3	33.5(12)	62.6(14)	54.4(13)	-7.0(11)	7.3(11)	5.1(11)
N1	33.1(15)	51.4(17)	37.9(14)	-8.0(12)	6.8(12)	2.7(13)
N2	29.1(13)	45.0(15)	35.9(13)	0.3(11)	5.7(11)	1.2(12)
N3	66(2)	43.7(16)	47.7(17)	-4.3(13)	16.9(16)	2.0(15)
C1	40.9(18)	46.8(18)	42.3(17)	-6.0(14)	8.8(15)	-0.3(15)
C2	36.9(17)	44.3(18)	38.6(16)	-2.9(14)	6.8(14)	-8.8(14)
C3	30.4(16)	47.3(18)	37.5(15)	-1.0(14)	3.1(14)	-1.7(14)
C4	40.6(18)	44.9(18)	41.7(17)	-0.3(14)	13.0(15)	3.9(15)
C5	53(2)	54(2)	65(2)	8.9(18)	9.8(19)	0.7(18)
C6	78(3)	49(2)	97(3)	10(2)	30(3)	-3(2)
C7	118(4)	50(2)	73(3)	17(2)	47(3)	16(3)
C8	113(4)	63(3)	49(2)	15.6(19)	9(2)	14(3)
C9	64(2)	61(2)	42.7(19)	-0.6(16)	0.2(18)	4.6(19)
C10	34.1(17)	40.0(17)	41.1(17)	-2.4(13)	10.3(15)	-3.0(14)
C11	37.6(18)	43.2(18)	39.1(16)	-3.9(13)	16.3(14)	0.5(14)
C12	51(2)	69(2)	49.0(19)	-4.0(17)	19.9(17)	-5.1(18)
C13	78(3)	91(3)	49(2)	4.9(19)	31(2)	5(2)
C14	68(3)	92(3)	38.4(19)	-8.0(19)	12.3(19)	12(2)
C15	50(2)	86(3)	54(2)	-25.9(19)	7.0(19)	-6(2)
C16	46(2)	59(2)	48.8(19)	-5.4(16)	13.7(17)	-9.4(17)
C17	69(3)	51(2)	58(2)	9.2(18)	7(2)	-2(2)

Table S4 Bond lengths for 3aa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C17	1.345(4)	C3	C4	1.505(4)
F2	C17	1.311(3)	C4	C5	1.384(4)
F3	C17	1.343(4)	C4	C9	1.377(4)
O1	N3	1.209(3)	C5	C6	1.385(5)
O2	N3	1.214(3)	C6	C7	1.367(5)
O3	C10	1.230(3)	C7	C8	1.370(5)
N1	N2	1.430(3)	C8	C9	1.382(5)
N1	C1	1.456(4)	C10	C11	1.491(4)
N2	C3	1.472(3)	C11	C12	1.377(4)
N2	C10	1.367(4)	C11	C16	1.386(4)
N3	C2	1.498(4)	C12	C13	1.386(4)
C1	C2	1.541(4)	C13	C14	1.370(5)
C1	C17	1.513(4)	C14	C15	1.371(5)
C2	C3	1.557(4)	C15	C16	1.383(4)

Table S5 Bond angles for 3aa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	N1	C1	104.3(2)	C6	C7	C8	120.0(4)
N1	N2	C3	112.2(2)	C7	C8	C9	120.0(3)
C10	N2	N1	118.9(2)	C4	C9	C8	121.0(3)
C10	N2	C3	119.3(2)	O3	C10	N2	120.5(3)
O1	N3	O2	125.0(3)	O3	C10	C11	121.4(3)
O1	N3	C2	118.5(3)	N2	C10	C11	118.0(2)
O2	N3	C2	116.5(3)	C12	C11	C10	119.5(3)
N1	C1	C2	107.0(2)	C12	C11	C16	119.4(3)
N1	C1	C17	110.2(3)	C16	C11	C10	120.8(3)
C17	C1	C2	110.3(2)	C11	C12	C13	120.2(3)
N3	C2	C1	110.7(2)	C14	C13	C12	120.2(4)
N3	C2	C3	111.8(2)	C13	C14	C15	119.8(3)
C1	C2	C3	105.0(2)	C14	C15	C16	120.5(3)
N2	C3	C2	102.7(2)	C15	C16	C11	119.8(3)
N2	C3	C4	113.8(2)	F1	C17	C1	110.0(3)
C4	C3	C2	116.3(3)	F2	C17	F1	107.2(3)
C5	C4	C3	122.5(3)	F2	C17	F3	107.9(3)
C9	C4	C3	119.3(3)	F2	C17	C1	112.5(3)
C9	C4	C5	118.3(3)	F3	C17	F1	106.4(3)
C4	C5	C6	120.7(3)	F3	C17	C1	112.5(3)
C7	C6	C5	120.0(4)				

Table S6 Torsion angles for 3aa.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	N3	C2	C1	-35.6(4)	C2	C1	C17	F1	62.6(4)
O1	N3	C2	C3	81.1(3)	C2	C1	C17	F2	-178.0(3)
O2	N3	C2	C1	145.7(3)	C2	C1	C17	F3	-55.9(4)
O2	N3	C2	C3	-97.6(3)	C2	C3	C4	C5	-91.4(3)
O3	C10	C11	C12	41.8(4)	C2	C3	C4	C9	88.5(3)
O3	C10	C11	C16	-131.9(3)	C3	N2	C10	O3	-8.8(4)
N1	N2	C3	C2	19.0(3)	C3	N2	C10	C11	176.0(2)
N1	N2	C3	C4	-107.6(3)	C3	C4	C5	C6	178.3(3)
N1	N2	C10	O3	-152.5(3)	C3	C4	C9	C8	-179.0(3)
N1	N2	C10	C11	32.2(4)	C4	C5	C6	C7	1.0(6)
N1	C1	C2	N3	103.8(3)	C5	C4	C9	C8	0.9(5)
N1	C1	C2	C3	-16.9(3)	C5	C6	C7	C8	0.2(6)
N1	C1	C17	F1	-179.4(3)	C6	C7	C8	C9	-0.9(6)
N1	C1	C17	F2	-60.0(4)	C7	C8	C9	C4	0.4(6)
N1	C1	C17	F3	62.1(3)	C9	C4	C5	C6	-1.6(5)
N2	N1	C1	C2	28.1(3)	C10	N2	C3	C2	-127.0(3)
N2	N1	C1	C17	-91.9(3)	C10	N2	C3	C4	106.5(3)
N2	C3	C4	C5	27.7(4)	C10	C11	C12	C13	-174.9(3)
N2	C3	C4	C9	-152.4(3)	C10	C11	C16	C15	173.0(3)
N2	C10	C11	C12	-143.0(3)	C11	C12	C13	C14	1.8(6)
N2	C10	C11	C16	43.3(4)	C12	C11	C16	C15	-0.7(5)
N3	C2	C3	N2	-120.7(2)	C12	C13	C14	C15	-0.7(6)
N3	C2	C3	C4	4.3(3)	C13	C14	C15	C16	-1.0(6)
C1	N1	N2	C3	-30.3(3)	C14	C15	C16	C11	1.7(5)
C1	N1	N2	C10	115.9(3)	C16	C11	C12	C13	-1.1(5)
C1	C2	C3	N2	-0.7(3)	C17	C1	C2	N3	-136.3(3)
C1	C2	C3	C4	124.3(3)	C17	C1	C2	C3	103.0(3)

Table S7 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) for 3aa.

Atom	*x*	*y*	*z*	U(eq)
H1	10910(60)	982(13)	7920(30)	69(12)
H1A	10529	201	7207	52
H2	6118	322	5969	48
H3	4863	1100	6396	47
H5	10321	1797	6729	69
H6	11135	2460	5532	88
H7	8460	2638	3850	91
H8	4958	2160	3359	91
H9	4172	1487	4531	69
H12	4557	1011	10232	66
H13	6126	1100	12172	84
H14	9780	1507	12797	79
H15	11916	1809	11491	77
H16	10466	1684	9552	61

5 X-ray Diffraction Structure of 4a

Figure S2. Diffraction Structure of 4a; thermal ellipsoids are set at a 50% probability level

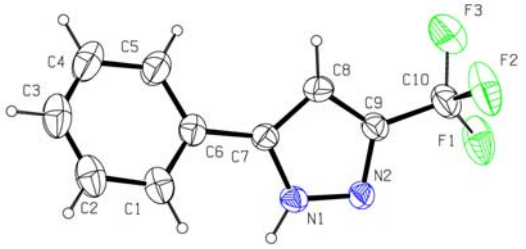


Table S8 Crystal data and structure refinement for 4a.

Identification code	PXS_2
Empirical formula	$C_{10}H_7F_3N_2$
Formula weight	212.18
Temperature/K	283(4)
Crystal system	triclinic
Space group	P-1
a/Å	9.9013(7)
b/Å	9.9393(8)
c/Å	21.0212(16)
α/°	80.533(7)
β/°	87.495(6)
γ/°	89.524(6)
Volume/Å^3	2038.6(3)
Z	8
ρ_{calc}g/cm^3	1.383
μ/mm^{-1}	0.123
F(000)	864.0
Crystal size/mm^3	0.22 × 0.17 × 0.04
Radiation	Mo Kα (λ = 0.7107)
2Θ range for data collection/°	6.766 to 52.044
Index ranges	-12 ≤ h ≤ 11, -12 ≤ k ≤ 11, -19 ≤ l ≤ 25
Reflections collected	13541
Independent reflections	8011 [R_{int} = 0.0367, R_{sigma} = 0.0686]
Data/restraints/parameters	8011/162/640
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0977, wR_2 = 0.2572
Final R indexes [all data]	R_1 = 0.1737, wR_2 = 0.3188
Largest diff. peak/hole / e Å^{-3}	0.32/-0.29

Table S9 Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for 4a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N3	4749(3)	7684(4)	1941.7(17)	68.2(10)
N4	5609(4)	6695(4)	1820.4(17)	70.3(10)
C21	2884(6)	10368(6)	923(3)	110(2)
C22	1921(9)	11383(8)	955(5)	140(3)
C23	1225(9)	11435(9)	1514(6)	144(3)
C24	1443(6)	10505(9)	2044(4)	122(2)
C25	2376(5)	9480(7)	2021(3)	97.7(17)
C26	3124(5)	9414(5)	1462(3)	80.9(14)
C27	4120(5)	8310(5)	1420(2)	68.5(11)
C28	4599(5)	7682(5)	918(2)	79.7(14)
C29	5506(5)	6708(5)	1193(2)	72.3(12)
C30	6284(7)	5702(8)	871(4)	103.6(19)
F7'	7313(17)	6310(20)	496(10)	154(6)
F8'	5688(19)	4960(20)	609(10)	139(6)
F9'	7050(20)	4900(20)	1336(8)	137(7)
N5	6279(3)	9466(4)	3073.0(16)	66.6(10)
N6	5210(4)	8638(4)	3134.6(17)	69.9(10)
C31	8231(6)	11662(8)	3110(4)	118(2)
C32	9261(7)	12562(9)	3160(6)	153(4)
C33	9763(9)	12685(13)	3736(9)	204(8)
C34	9277(11)	11878(15)	4259(7)	192(6)
C35	8232(8)	10954(9)	4245(4)	146(3)
C36	7712(5)	10840(7)	3652(3)	93.3(18)
C37	6591(5)	9892(5)	3626(2)	74.6(14)
C38	5664(5)	9280(7)	4076(2)	90.7(17)
C39	4850(5)	8527(6)	3749(2)	80.8(14)
C40	3660(8)	7659(10)	4002(3)	113(2)
F10'	4050(20)	6460(20)	4331(13)	163(8)
F11'	2780(20)	7590(30)	3595(13)	222(9)
F12'	3060(20)	8150(20)	4470(10)	180(7)
N7	8650(3)	8241(4)	1989.4(16)	66.5(9)
N8	7839(4)	9343(4)	1902.6(16)	69.3(10)
C11	10887(6)	6279(6)	2017(4)	112(2)
C12	11855(7)	5249(8)	2018(5)	132(2)
C13	12231(9)	4928(9)	1443(6)	153(3)

C14	11759(9)	5454(10)	891(5)	153(3)
C15	10747(7)	6536(7)	871(3)	121(2)
C16	10331(5)	6921(6)	1453(3)	86.3(15)
C17	9360(5)	8042(5)	1453(2)	73.6(12)
C18	8977(5)	9094(6)	983(2)	83.7(14)
C19	8061(5)	9854(5)	1288(2)	74.4(12)
C20	7346(9)	11125(8)	1014(4)	110(2)
F4'	7930(20)	11627(17)	430(7)	187(6)
F5'	6173(15)	11051(17)	927(12)	174(6)
F6'	7560(20)	12080(15)	1353(9)	175(5)
N1	6876(4)	5591(4)	2994.0(16)	67.2(10)
N2	7893(3)	6376(4)	3126.2(17)	68.4(10)
C1	5065(6)	3298(6)	2891(3)	95.5(17)
C2	4035(7)	2353(7)	2874(4)	112(2)
C3	3258(7)	1898(7)	3394(5)	118(2)
C4	3431(6)	2345(8)	3958(4)	121(2)
C5	4448(5)	3273(7)	3997(3)	99.8(17)
C6	5276(5)	3772(5)	3467(3)	75.8(13)
C7	6370(4)	4732(5)	3511(2)	65.9(11)
C8	7125(5)	4987(6)	4018(2)	79.0(14)
C9	8022(4)	5982(5)	3759(2)	70.2(12)
C10	9063(6)	6653(8)	4089(3)	98.6(18)
F1'	9880(20)	7420(30)	3670(12)	169(9)
F2'	8556(11)	7239(14)	4562(6)	139(4)
F5	5604(15)	4481(12)	941(6)	143(5)
F1	9382(12)	7855(9)	3815(7)	139(4)
F9	6338(14)	11443(13)	1456(5)	132(4)
F3	8898(15)	6374(16)	4711(6)	164(5)
F7	8083(13)	12164(13)	879(11)	145(4)
F11	2543(8)	8450(10)	4013(7)	139(3)
F2	10137(5)	5899(5)	4187(3)	168.6(19)
F4	7441(12)	5417(16)	1087(8)	152(5)
F6	6400(18)	6112(15)	241(4)	175(4)
F8	6547(19)	10908(17)	550(6)	149(6)
F10	3750(17)	6970(20)	4547(6)	190(6)
F12	3324(9)	6793(9)	3596(5)	125(3)

Table S10 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N3	72(2)	69(2)	67(2)	-18.4(18)	-9.5(17)	-2.1(19)
N4	74(2)	67(2)	71(2)	-11.6(18)	-11.2(17)	3.7(19)
C21	110(4)	78(4)	140(5)	-3(4)	-33(4)	9(4)
C22	123(6)	82(5)	213(9)	-9(6)	-58(6)	12(5)
C23	112(6)	83(5)	249(11)	-51(7)	-51(7)	9(5)
C24	86(4)	122(6)	176(7)	-80(6)	-20(4)	8(4)
C25	74(3)	100(5)	130(5)	-49(4)	-7(3)	-2(3)
C26	75(3)	57(3)	116(4)	-22(3)	-26(3)	-6(2)
C27	76(3)	58(3)	72(3)	-8(2)	-20(2)	-4(2)
C28	95(3)	80(4)	65(3)	-11(2)	-18(2)	4(3)
C29	79(3)	73(3)	67(3)	-17(2)	-8(2)	0(2)
C30	101(5)	109(6)	109(5)	-41(4)	-17(4)	13(4)
F7'	141(10)	181(12)	143(11)	-52(10)	61(9)	-4(9)
F8'	137(9)	145(14)	162(13)	-108(12)	-5(9)	-31(9)
F9'	168(15)	127(11)	117(8)	-26(7)	-7(8)	73(11)
N5	65(2)	71(3)	65(2)	-17.8(18)	2.4(16)	-1.5(19)
N6	68(2)	75(3)	69(2)	-16.0(19)	-1.4(17)	-7(2)
C31	69(3)	110(6)	190(7)	-76(5)	10(4)	-8(3)
C32	84(4)	132(7)	265(11)	-112(7)	40(5)	-36(4)
C33	74(5)	153(11)	430(20)	-188(14)	-8(8)	-5(5)
C34	124(8)	208(14)	297(16)	-174(13)	-96(9)	21(8)
C35	131(6)	157(8)	179(7)	-94(6)	-72(5)	26(5)
C36	64(3)	96(5)	135(5)	-64(4)	-16(3)	10(3)
C37	70(3)	89(4)	73(3)	-36(3)	-15(2)	19(3)
C38	88(3)	127(5)	64(3)	-37(3)	0(3)	7(3)
C39	83(3)	102(4)	57(3)	-13(3)	3(2)	6(3)
C40	102(5)	145(8)	86(5)	-7(5)	12(4)	-12(5)
F10'	159(11)	123(10)	199(16)	-23(10)	62(10)	-15(9)
F11'	182(15)	256(19)	220(15)	-13(15)	7(13)	-83(14)
F12'	169(12)	173(13)	181(12)	-15(10)	116(10)	9(10)
N7	70(2)	63(2)	63(2)	0.2(17)	5.7(16)	-3.3(18)
N8	72(2)	63(2)	71(2)	-7.8(18)	1.1(17)	-1.7(19)
C11	84(4)	69(4)	178(6)	-8(4)	20(4)	6(3)
C12	106(4)	98(5)	183(6)	-3(5)	17(4)	-2(4)
C13	132(6)	110(6)	219(8)	-47(6)	35(6)	-11(5)

C14	138(6)	154(7)	183(6)	-87(6)	50(5)	-12(5)
C15	113(4)	112(5)	145(5)	-53(4)	35(4)	-6(4)
C16	74(3)	67(3)	120(4)	-27(3)	26(3)	-12(3)
C17	76(3)	63(3)	82(3)	-21(2)	18(2)	-15(2)
C18	106(4)	81(4)	62(3)	-9(3)	14(2)	-13(3)
C19	85(3)	66(3)	67(3)	3(2)	1(2)	-6(2)
C20	124(6)	95(6)	103(5)	10(4)	-21(4)	0(5)
F4'	230(13)	148(10)	144(8)	87(7)	18(9)	31(9)
F5'	118(8)	157(10)	229(15)	32(13)	-30(12)	15(7)
F6'	236(14)	93(8)	199(11)	-25(9)	-58(11)	48(9)
N1	74(2)	63(2)	62(2)	-0.2(17)	-12.4(16)	-0.6(19)
N2	68(2)	64(2)	71(2)	-1.9(18)	-10.2(17)	-9.1(18)
C1	86(3)	84(4)	119(4)	-20(3)	-26(3)	3(3)
C2	101(4)	83(5)	157(6)	-28(4)	-41(4)	0(4)
C3	88(4)	82(5)	184(8)	-11(5)	-29(5)	-10(3)
C4	84(4)	106(6)	162(7)	11(5)	11(4)	-19(4)
C5	84(3)	97(5)	112(4)	-2(3)	5(3)	-16(3)
C6	65(3)	62(3)	97(3)	1(3)	-14(2)	5(2)
C7	62(2)	67(3)	66(3)	1(2)	-5.0(19)	5(2)
C8	81(3)	86(4)	64(3)	7(2)	-5(2)	-2(3)
C9	69(3)	71(3)	69(3)	-5(2)	-15(2)	0(2)
C10	91(4)	101(5)	102(4)	-3(4)	-38(4)	-2(4)
F1'	136(13)	223(19)	145(11)	-10(14)	-26(10)	-88(13)
F2'	134(7)	172(9)	140(8)	-99(8)	-36(6)	2(7)
F5	164(8)	82(6)	189(10)	-47(6)	26(7)	10(5)
F1	136(8)	69(4)	217(12)	-13(5)	-79(7)	-19(4)
F9	135(7)	128(8)	122(6)	5(5)	15(6)	65(6)
F3	169(8)	201(9)	129(7)	-32(7)	-47(6)	-37(7)
F7	140(7)	77(6)	200(12)	29(8)	-5(9)	-1(6)
F11	79(4)	125(6)	210(9)	-21(7)	26(5)	-13(4)
F2	130(3)	136(4)	251(5)	-40(4)	-99(3)	3(3)
F4	98(6)	165(12)	217(15)	-102(10)	-18(8)	25(7)
F6	255(12)	175(10)	100(6)	-47(6)	37(7)	50(9)
F8	179(13)	168(10)	99(6)	-2(7)	-63(7)	42(9)
F10	191(11)	218(14)	125(8)	74(9)	16(7)	-33(10)
F12	124(6)	112(6)	144(6)	-44(5)	31(4)	-49(4)

Table S11 Bond Lengths for 4a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N3	N4	1.344(5)	N7	N8	1.346(5)
N3	C27	1.344(5)	N7	C17	1.344(5)
N4	C29	1.325(5)	N8	C19	1.319(5)
C21	C22	1.390(9)	C11	C12	1.396(8)
C21	C26	1.381(7)	C11	C16	1.384(8)
C22	C23	1.345(11)	C12	C13	1.336(11)
C23	C24	1.348(11)	C13	C14	1.297(11)
C24	C25	1.375(8)	C14	C15	1.460(11)
C25	C26	1.373(7)	C15	C16	1.387(7)
C26	C27	1.479(6)	C16	C17	1.466(7)
C27	C28	1.376(6)	C17	C18	1.377(7)
C28	C29	1.387(6)	C18	C19	1.378(6)
C29	C30	1.489(7)	C19	C20	1.487(8)
C30	F7'	1.347(16)	C20	F4'	1.354(14)
C30	F8'	1.169(17)	C20	F5'	1.188(15)
C30	F9'	1.399(19)	C20	F6'	1.299(15)
C30	F5	1.376(14)	C20	F9	1.404(12)
C30	F4	1.263(14)	C20	F7	1.256(14)
C30	F6	1.322(11)	C20	F8	1.329(16)
N5	N6	1.335(5)	N1	N2	1.345(5)
N5	C37	1.350(5)	N1	C7	1.348(5)
N6	C39	1.311(5)	N2	C9	1.335(5)
C31	C32	1.382(10)	C1	C2	1.398(9)
C31	C36	1.370(9)	C1	C6	1.394(7)
C32	C33	1.352(15)	C2	C3	1.327(9)
C33	C34	1.325(18)	C3	C4	1.351(9)
C34	C35	1.394(14)	C4	C5	1.385(9)
C35	C36	1.392(8)	C5	C6	1.380(7)
C36	C37	1.471(8)	C6	C7	1.465(7)
C37	C38	1.360(7)	C7	C8	1.386(6)
C38	C39	1.382(7)	C8	C9	1.363(7)
C39	C40	1.493(9)	C9	C10	1.488(8)
C40	F10'	1.34(2)	C10	F1'	1.32(3)
C40	F11'	1.25(2)	C10	F2'	1.312(12)
C40	F12'	1.292(15)	C10	F1	1.273(12)
C40	F11	1.354(12)	C10	F3	1.295(14)

C40	F10	1.239(14)	C10	F2	1.300(7)
C40	F12	1.360(12)	F3	F2	1.727(16)

Table S12 Bond Angles for 4a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N4	N3	C27	114.0(3)	C17	N7	N8	113.8(4)
C29	N4	N3	103.0(3)	C19	N8	N7	103.3(3)
C26	C21	C22	120.2(7)	C16	C11	C12	122.0(7)
C23	C22	C21	119.7(8)	C13	C12	C11	116.3(8)
C22	C23	C24	120.7(8)	C14	C13	C12	126.3(9)
C23	C24	C25	120.7(8)	C13	C14	C15	118.9(8)
C26	C25	C24	120.2(7)	C16	C15	C14	117.2(7)
C21	C26	C27	120.0(5)	C11	C16	C15	119.2(6)
C25	C26	C21	118.5(5)	C11	C16	C17	121.6(5)
C25	C26	C27	121.4(5)	C15	C16	C17	119.1(6)
N3	C27	C26	121.7(4)	N7	C17	C16	122.1(5)
N3	C27	C28	105.3(4)	N7	C17	C18	104.8(4)
C28	C27	C26	132.9(4)	C18	C17	C16	133.1(4)
C27	C28	C29	104.9(4)	C17	C18	C19	105.5(4)
N4	C29	C28	112.7(4)	N8	C19	C18	112.5(4)
N4	C29	C30	119.6(4)	N8	C19	C20	118.8(5)
C28	C29	C30	127.7(5)	C18	C19	C20	128.7(5)
F7'	C30	C29	110.7(9)	F4'	C20	C19	108.9(8)
F7'	C30	F9'	98.3(13)	F5'	C20	C19	117.9(11)
F8'	C30	C29	118.4(10)	F5'	C20	F4'	105.5(13)
F8'	C30	F7'	111.9(13)	F5'	C20	F6'	109.9(15)
F8'	C30	F9'	107.4(16)	F6'	C20	C19	110.3(8)
F9'	C30	C29	108.0(9)	F6'	C20	F4'	103.2(14)
F5	C30	C29	110.9(8)	F9	C20	C19	110.2(6)
F4	C30	C29	114.7(8)	F7	C20	C19	114.9(8)
F4	C30	F5	105.8(11)	F7	C20	F9	106.1(12)
F4	C30	F6	109.4(11)	F7	C20	F8	115.1(12)
F6	C30	C29	110.9(7)	F8	C20	C19	111.0(9)
F6	C30	F5	104.5(10)	F8	C20	F9	98.0(11)
N6	N5	C37	113.9(4)	N2	N1	C7	114.0(4)
C39	N6	N5	103.2(4)	C9	N2	N1	103.0(4)
C36	C31	C32	119.9(8)	C6	C1	C2	119.1(6)
C33	C32	C31	121.8(11)	C3	C2	C1	121.4(7)
C34	C33	C32	118.4(11)	C2	C3	C4	120.9(7)
C33	C34	C35	122.8(12)	C3	C4	C5	119.5(7)
C36	C35	C34	118.5(10)	C6	C5	C4	121.4(6)

C31	C36	C35	118.5(7)	C1	C6	C7	120.9(5)
C31	C36	C37	122.0(5)	C5	C6	C1	117.7(5)
C35	C36	C37	119.5(7)	C5	C6	C7	121.4(5)
N5	C37	C36	122.0(5)	N1	C7	C6	122.5(4)
N5	C37	C38	104.8(5)	N1	C7	C8	104.6(4)
C38	C37	C36	133.2(5)	C8	C7	C6	132.9(4)
C37	C38	C39	105.5(4)	C9	C8	C7	105.9(4)
N6	C39	C38	112.6(5)	N2	C9	C8	112.6(4)
N6	C39	C40	118.7(5)	N2	C9	C10	118.7(5)
C38	C39	C40	128.7(5)	C8	C9	C10	128.6(5)
F10'	C40	C39	111.3(12)	F1'	C10	C9	111.4(12)
F11'	C40	C39	114.2(11)	F2'	C10	C9	113.2(7)
F11'	C40	F10'	115(2)	F2'	C10	F1'	115.4(14)
F11'	C40	F12'	106.2(17)	F1	C10	C9	114.7(7)
F12'	C40	C39	109.4(11)	F1	C10	F3	120.4(11)
F12'	C40	F10'	98.9(13)	F1	C10	F2	110.6(8)
F11	C40	C39	109.5(8)	F3	C10	C9	111.8(8)
F11	C40	F12	102.4(9)	F3	C10	F2	83.5(8)
F10	C40	C39	116.4(9)	F2	C10	C9	111.8(6)
F10	C40	F11	107.8(11)	C10	F3	F2	48.4(6)
F10	C40	F12	107.4(13)	C10	F2	F3	48.1(5)
F12	C40	C39	112.3(6)				

Table S13 Torsion Angles for 4a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N3	N4	C29	C28	0.0(6)	N7	N8	C19	C20	-178.7(6)
N3	N4	C29	C30	-177.8(5)	N7	C17	C18	C19	0.5(6)
N3	C27	C28	C29	-0.3(5)	N8	N7	C17	C16	178.0(4)
N4	N3	C27	C26	179.3(4)	N8	N7	C17	C18	-0.1(5)
N4	N3	C27	C28	0.3(5)	N8	C19	C20	F4'	166.8(13)
N4	C29	C30	F7'	-107.7(13)	N8	C19	C20	F5'	-73.2(18)
N4	C29	C30	F8'	121.0(16)	N8	C19	C20	F6'	54.1(17)
N4	C29	C30	F9'	-1.2(14)	N8	C19	C20	F9	-10.5(13)
N4	C29	C30	F5	83.9(9)	N8	C19	C20	F7	109.3(14)
N4	C29	C30	F4	-35.9(13)	N8	C19	C20	F8	-118.0(11)
N4	C29	C30	F6	-160.5(11)	C11	C12	C13	C14	-1.9(14)
C21	C22	C23	C24	-0.6(13)	C11	C16	C17	N7	-20.5(8)
C21	C26	C27	N3	155.3(5)	C11	C16	C17	C18	156.9(6)
C21	C26	C27	C28	-26.0(8)	C12	C11	C16	C15	-0.2(9)
C22	C21	C26	C25	1.1(9)	C12	C11	C16	C17	-177.3(6)
C22	C21	C26	C27	178.1(6)	C12	C13	C14	C15	2.1(16)
C22	C23	C24	C25	-0.4(12)	C13	C14	C15	C16	-1.1(12)
C23	C24	C25	C26	1.7(10)	C14	C15	C16	C11	0.2(9)
C24	C25	C26	C21	-2.1(8)	C14	C15	C16	C17	177.4(6)
C24	C25	C26	C27	-179.0(5)	C15	C16	C17	N7	162.3(5)
C25	C26	C27	N3	-27.8(7)	C15	C16	C17	C18	-20.2(9)
C25	C26	C27	C28	150.9(6)	C16	C11	C12	C13	0.9(11)
C26	C21	C22	C23	0.2(11)	C16	C17	C18	C19	-177.3(5)
C26	C27	C28	C29	-179.1(5)	C17	N7	N8	C19	-0.4(5)
C27	N3	N4	C29	-0.2(5)	C17	C18	C19	N8	-0.8(6)
C27	C28	C29	N4	0.2(6)	C17	C18	C19	C20	178.5(7)
C27	C28	C29	C30	177.7(6)	C18	C19	C20	F4'	-12.5(17)
C28	C29	C30	F7'	74.9(14)	C18	C19	C20	F5'	107.5(17)
C28	C29	C30	F8'	-56.3(19)	C18	C19	C20	F6'	-125.1(15)
C28	C29	C30	F9'	-178.5(12)	C18	C19	C20	F9	170.2(10)
C28	C29	C30	F5	-93.5(10)	C18	C19	C20	F7	-70.0(16)
C28	C29	C30	F4	146.7(11)	C18	C19	C20	F8	62.8(14)
C28	C29	C30	F6	22.2(14)	N1	N2	C9	C8	0.1(5)
N5	N6	C39	C38	0.5(5)	N1	N2	C9	C10	-179.3(4)
N5	N6	C39	C40	180.0(5)	N1	C7	C8	C9	0.0(5)
N5	C37	C38	C39	-0.4(5)	N2	N1	C7	C6	-178.8(4)

N6	N5	C37	C36	-178.3(4)	N2	N1	C7	C8	0.0(5)
N6	N5	C37	C38	0.8(5)	N2	C9	C10	F1'	-10.3(15)
N6	C39	C40	F10'	103.3(13)	N2	C9	C10	F2'	121.7(9)
N6	C39	C40	F11'	-30(2)	N2	C9	C10	F1	25.6(11)
N6	C39	C40	F12'	-148.4(14)	N2	C9	C10	F3	167.2(9)
N6	C39	C40	F11	-96.1(10)	N2	C9	C10	F2	-101.2(6)
N6	C39	C40	F10	141.4(13)	C1	C2	C3	C4	0.6(10)
N6	C39	C40	F12	17.0(11)	C1	C6	C7	N1	26.0(6)
C31	C32	C33	C34	2.4(16)	C1	C6	C7	C8	-152.4(5)
C31	C36	C37	N5	20.5(7)	C2	C1	C6	C5	0.2(7)
C31	C36	C37	C38	-158.2(6)	C2	C1	C6	C7	178.2(4)
C32	C31	C36	C35	1.0(8)	C2	C3	C4	C5	-1.1(10)
C32	C31	C36	C37	178.3(5)	C3	C4	C5	C6	1.2(10)
C32	C33	C34	C35	-2.9(18)	C4	C5	C6	C1	-0.8(8)
C33	C34	C35	C36	2.4(15)	C4	C5	C6	C7	-178.7(5)
C34	C35	C36	C31	-1.4(9)	C5	C6	C7	N1	-156.1(4)
C34	C35	C36	C37	-178.8(6)	C5	C6	C7	C8	25.5(7)
C35	C36	C37	N5	-162.2(5)	C6	C1	C2	C3	-0.2(9)
C35	C36	C37	C38	19.1(8)	C6	C7	C8	C9	178.6(4)
C36	C31	C32	C33	-1.5(11)	C7	N1	N2	C9	-0.1(4)
C36	C37	C38	C39	178.5(5)	C7	C8	C9	N2	-0.1(5)
C37	N5	N6	C39	-0.8(5)	C7	C8	C9	C10	179.2(5)
C37	C38	C39	N6	-0.1(6)	C8	C9	C10	F1'	170.5(14)
C37	C38	C39	C40	-179.5(6)	C8	C9	C10	F2'	-57.5(11)
C38	C39	C40	F10'	-77.4(15)	C8	C9	C10	F1	-153.6(9)
C38	C39	C40	F11'	150(2)	C8	C9	C10	F3	-12.0(12)
C38	C39	C40	F12'	30.9(17)	C8	C9	C10	F2	79.6(8)
C38	C39	C40	F11	83.2(11)	C9	C10	F3	F2	110.9(7)
C38	C39	C40	F10	-39.3(17)	C9	C10	F2	F3	-110.9(9)
C38	C39	C40	F12	-163.7(8)	F1	C10	F3	F2	-110.0(10)
N7	N8	C19	C18	0.7(5)	F1	C10	F2	F3	120.1(11)

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4a.

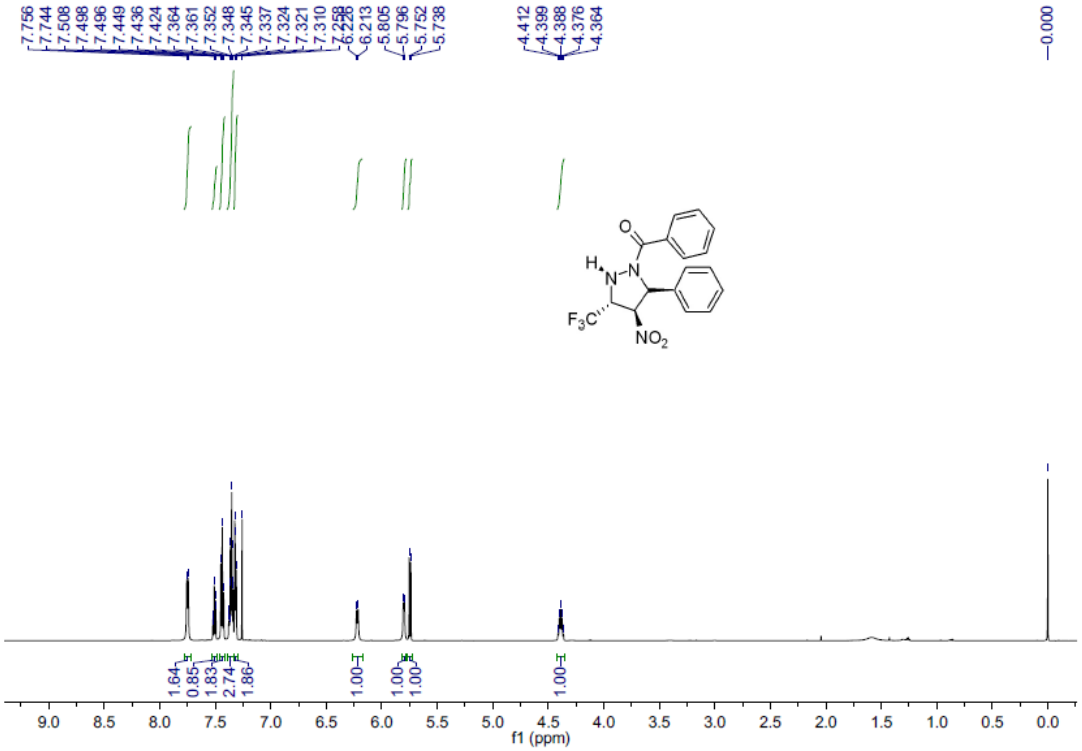
Atom	*x*	*y*	*z*	U(eq)
H3	4612	7897	2320	82
H21	3368	10332	537	132
H22	1759	12024	591	167
H23	587	12120	1536	173
H24	957	10558	2428	146
H25	2500	8830	2386	117
H28	4366	7870	489	96
H5	6729	9706	2713	80
H31	7889	11613	2710	141
H32	9620	13099	2788	183
H33	10434	13320	3764	245
H34	9649	11931	4653	231
H35	7890	10425	4624	176
H38	5594	9352	4512	109
H7	8709	7712	2355	80
H11	10607	6541	2406	135
H12	12218	4810	2398	158
H13	12896	4263	1439	183
H14	12061	5148	515	184
H15	10396	6949	483	145
H18	9275	9258	552	100
H1	6575	5633	2613	81
H1A	5603	3606	2523	115
H2	3891	2037	2490	134
H3A	2585	1263	3370	142
H4	2871	2032	4318	146
H5A	4575	3565	4388	120
H8	7038	4566	4447	95

Table S15 Atomic Occupancy for 4a.

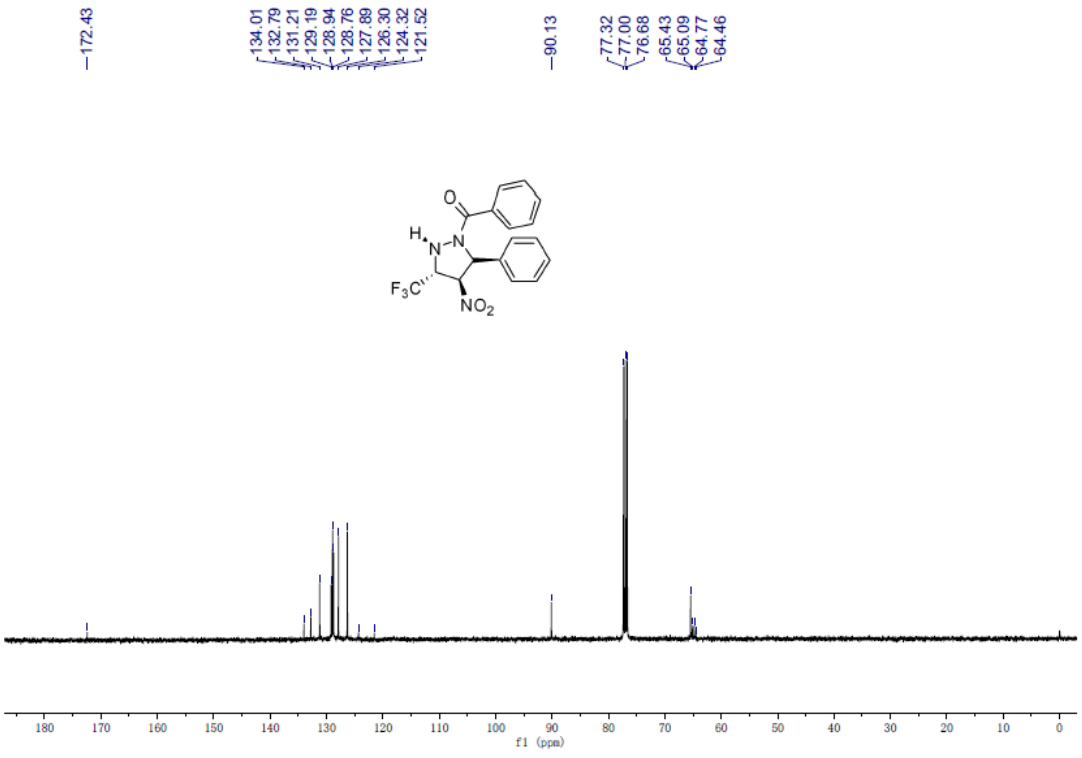
Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
F7'	0.4	F8'	0.4	F9'	0.4
F10'	0.4	F11'	0.4	F12'	0.4
F4'	0.5	F5'	0.5	F6'	0.5
F1'	0.35	F2'	0.5	F5	0.6
F1	0.65	F9	0.5	F3	0.5
F7	0.5	F11	0.6	F4	0.6
F6	0.6	F8	0.5	F10	0.6
F12	0.6				

6 NMR, HRMS copies of compounds 3aa-3sa

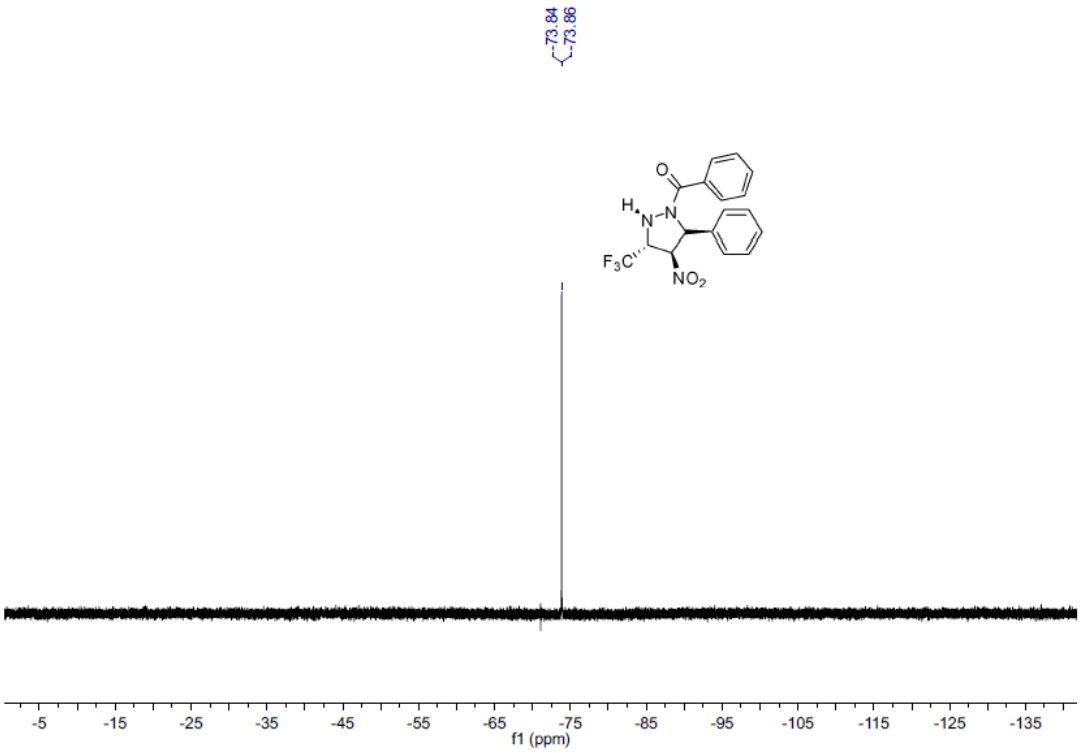
^{1}H NMR copies of compound **3aa**:



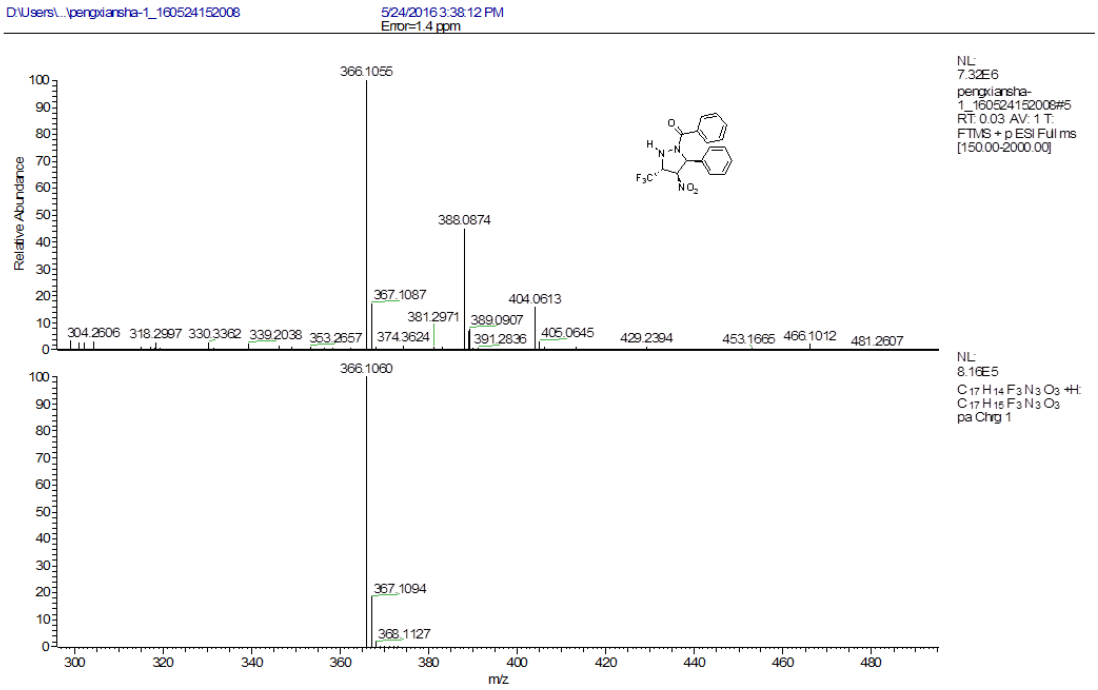
^{13}C NMR copies of compound **3aa**:



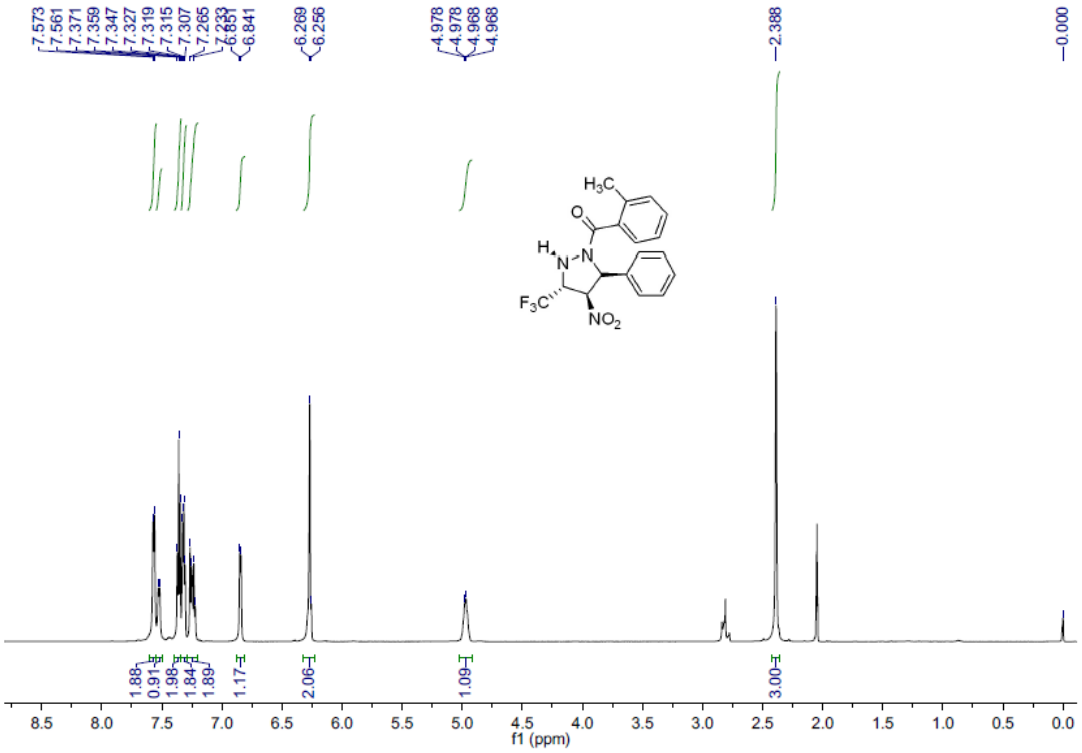
^{19}F NMR copies of compound **3aa**:



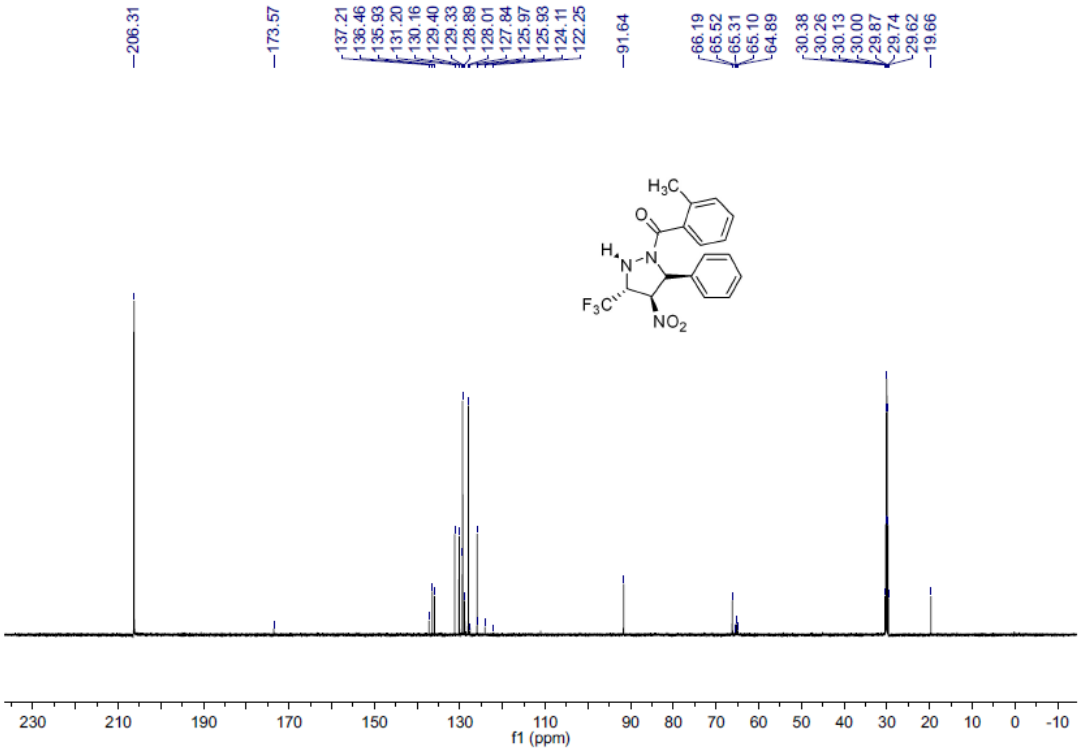
HRMS (ESI) of compound **3aa**:



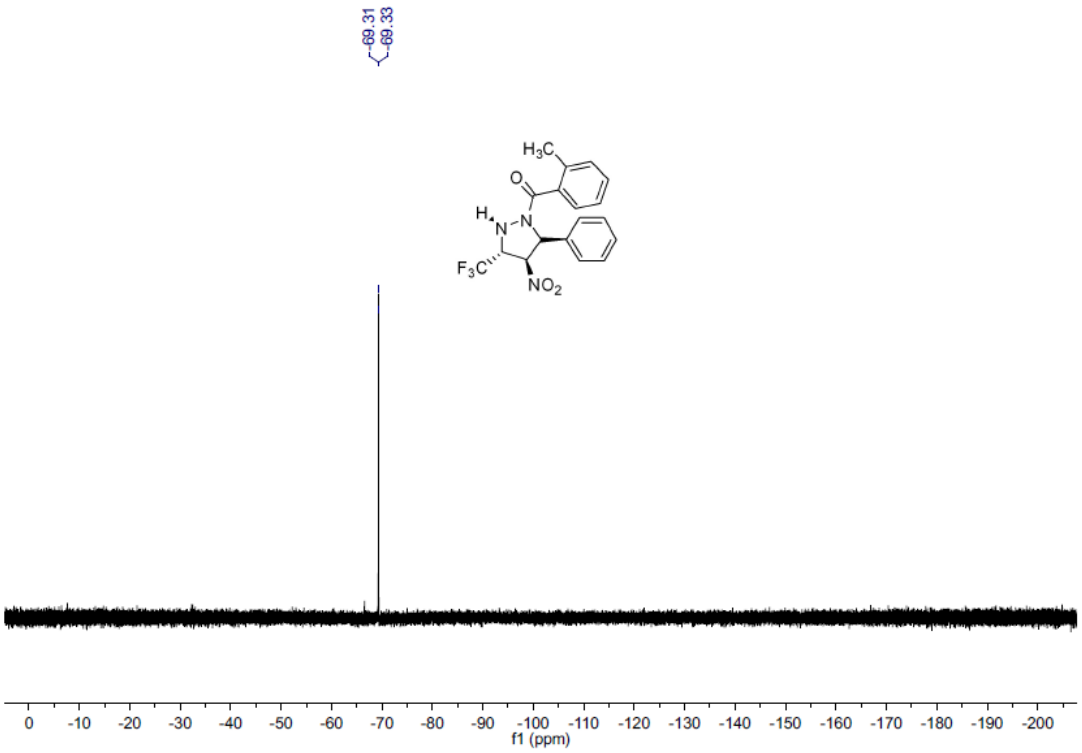
^{1}H NMR copies of compound **3ba**:



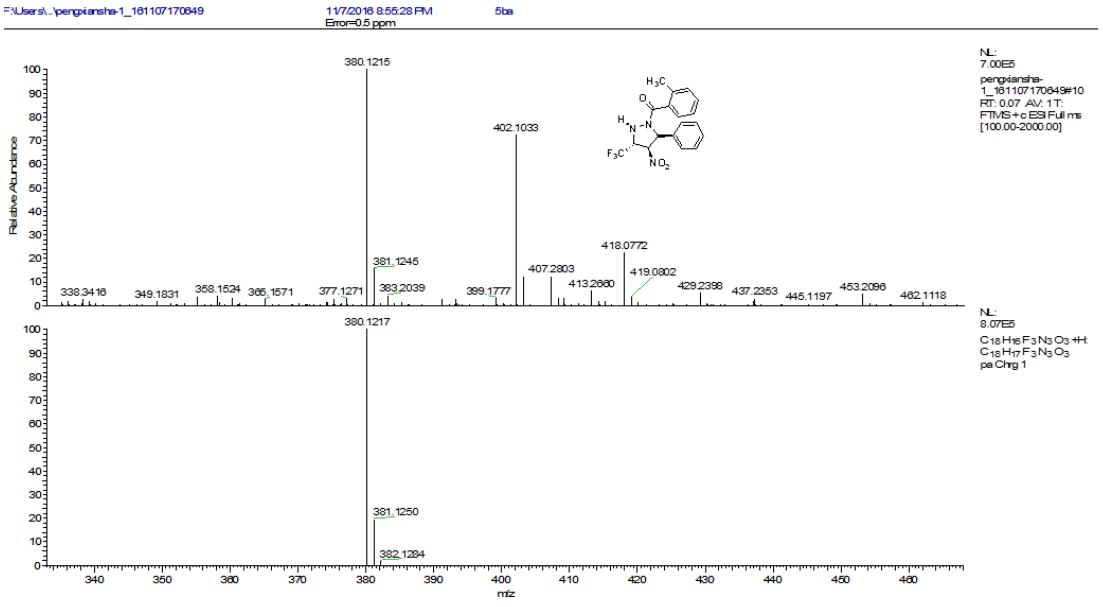
^{13}C NMR copies of compound **3ba**:



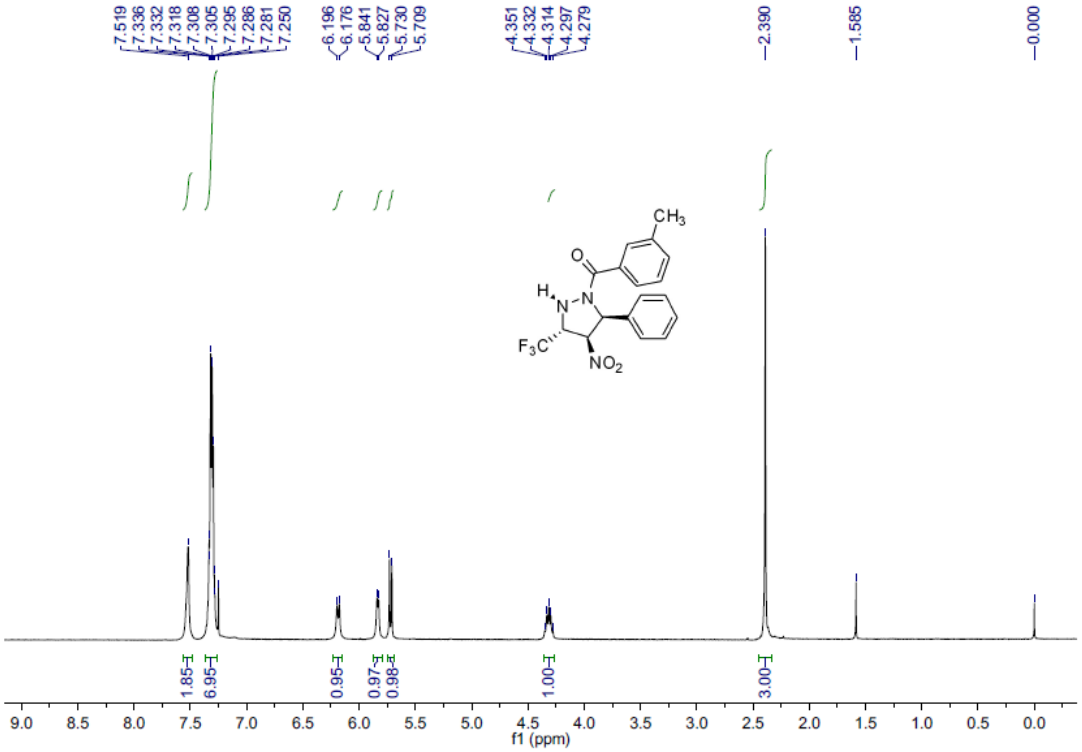
^{19}F NMR copies of compound **3ba**:



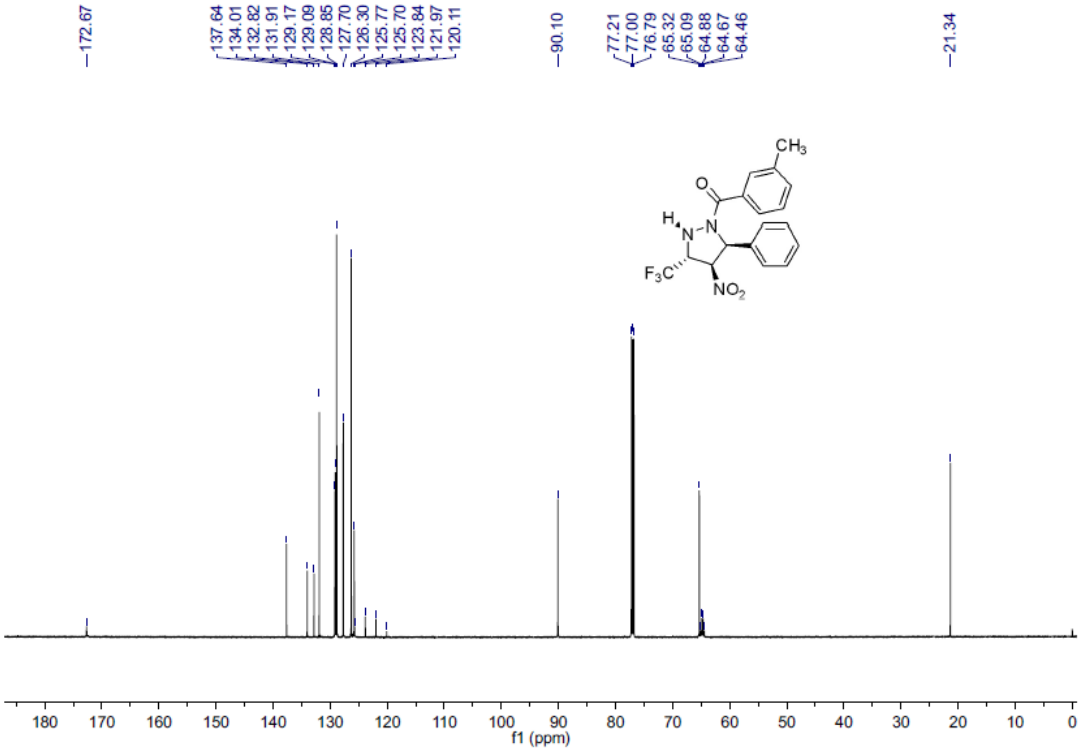
HRMS (ESI) of compound **3ba**:



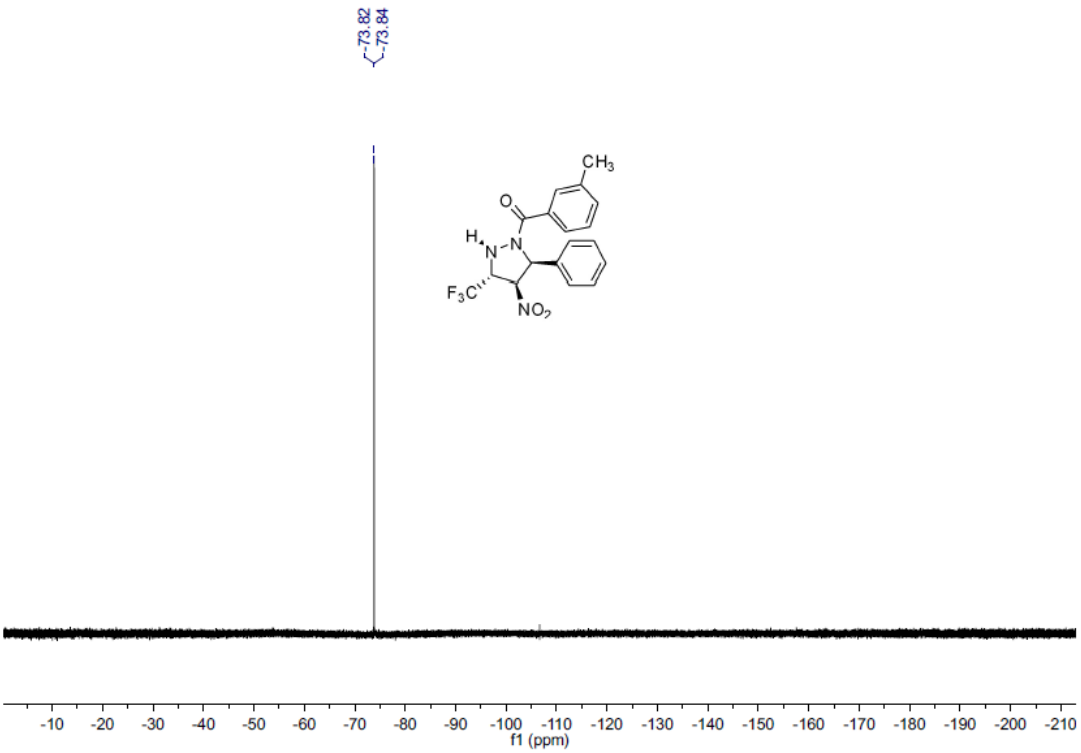
^{1}H NMR copies of compound **3ca**:



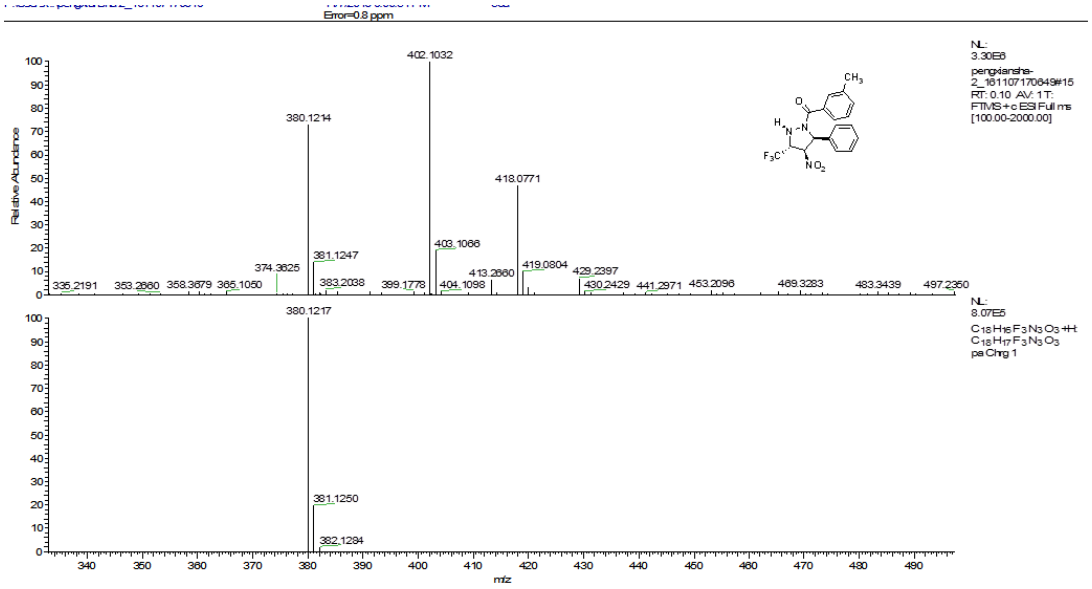
^{13}C NMR copies of compound **3ca**:



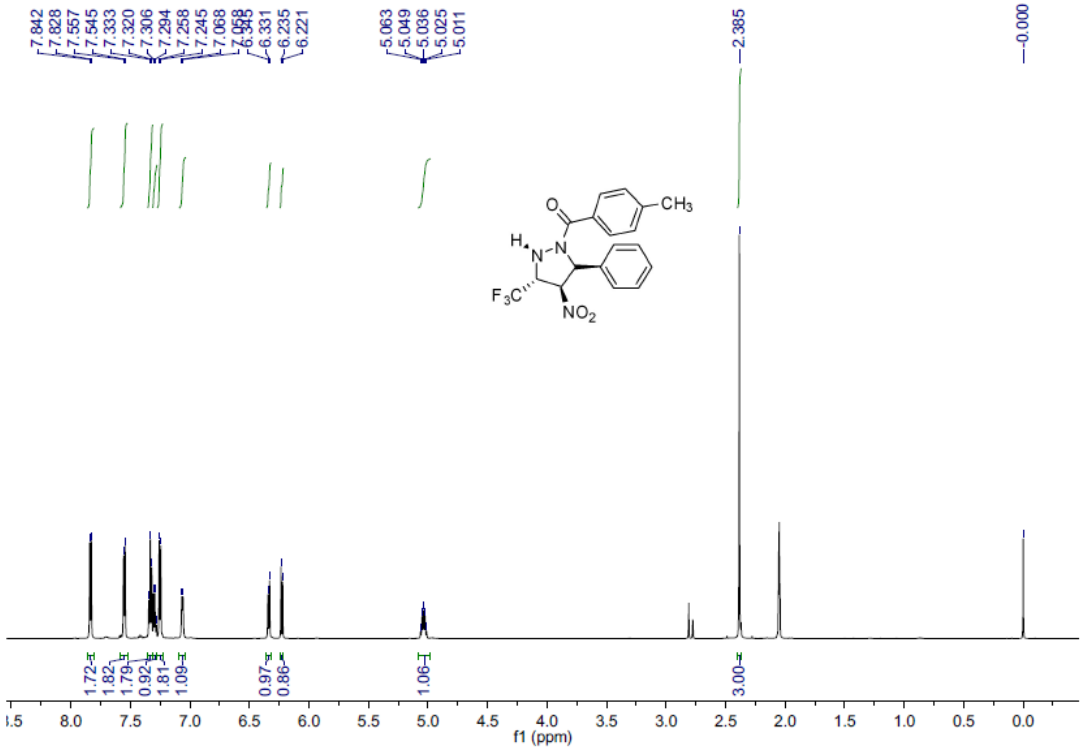
^{19}F NMR copies of compound **3ca**:



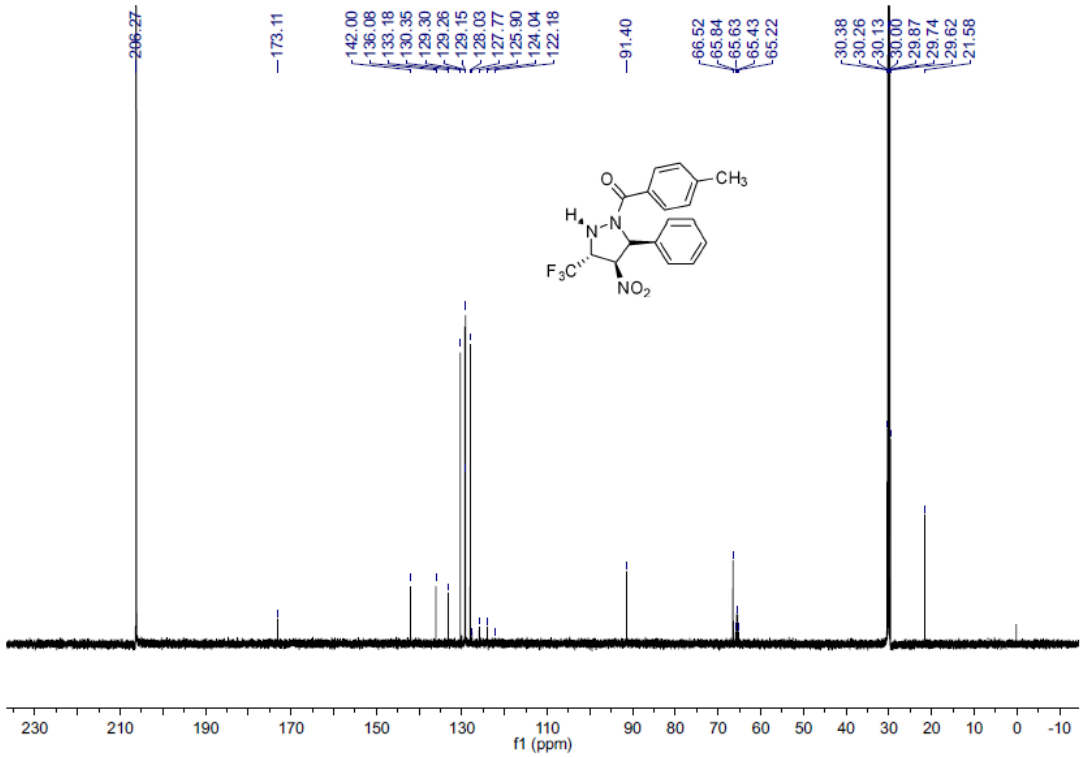
HRMS (ESI) of compound **3ca**:



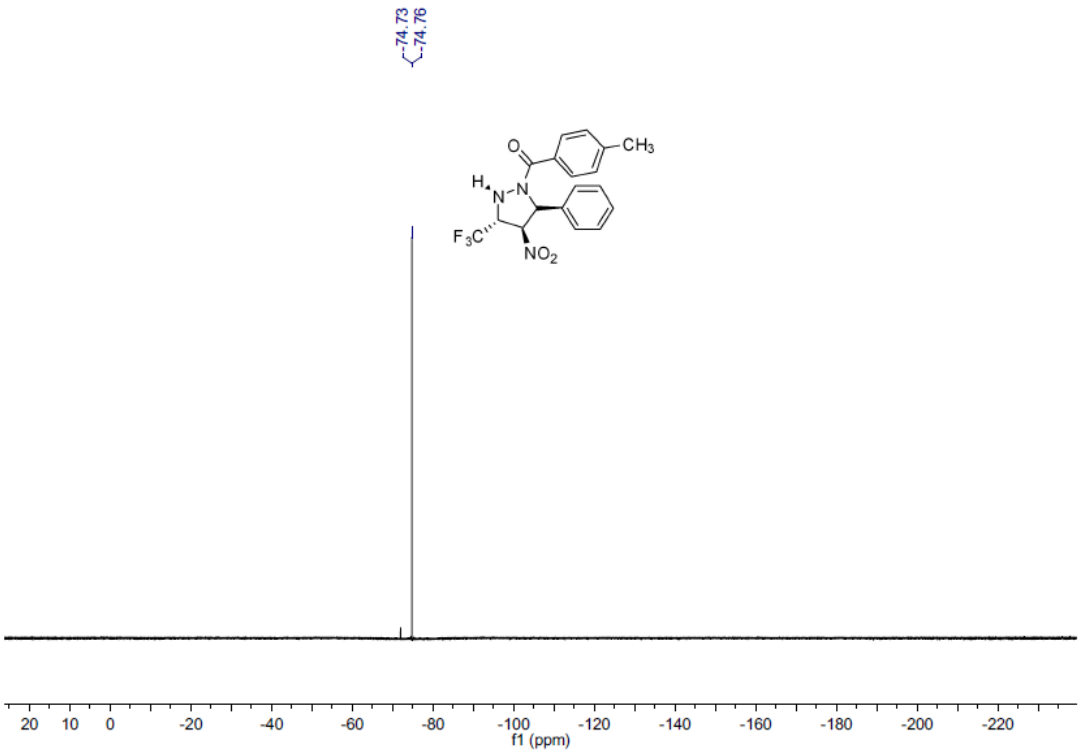
^{1}H NMR copies of compound **3da**:



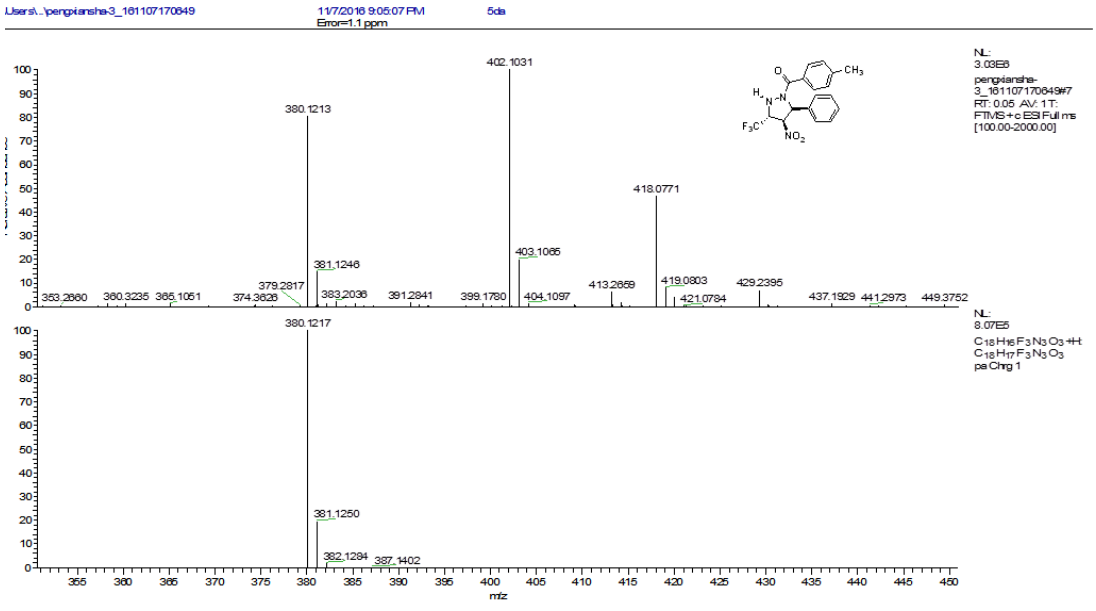
^{13}C NMR copies of compound **3da**:



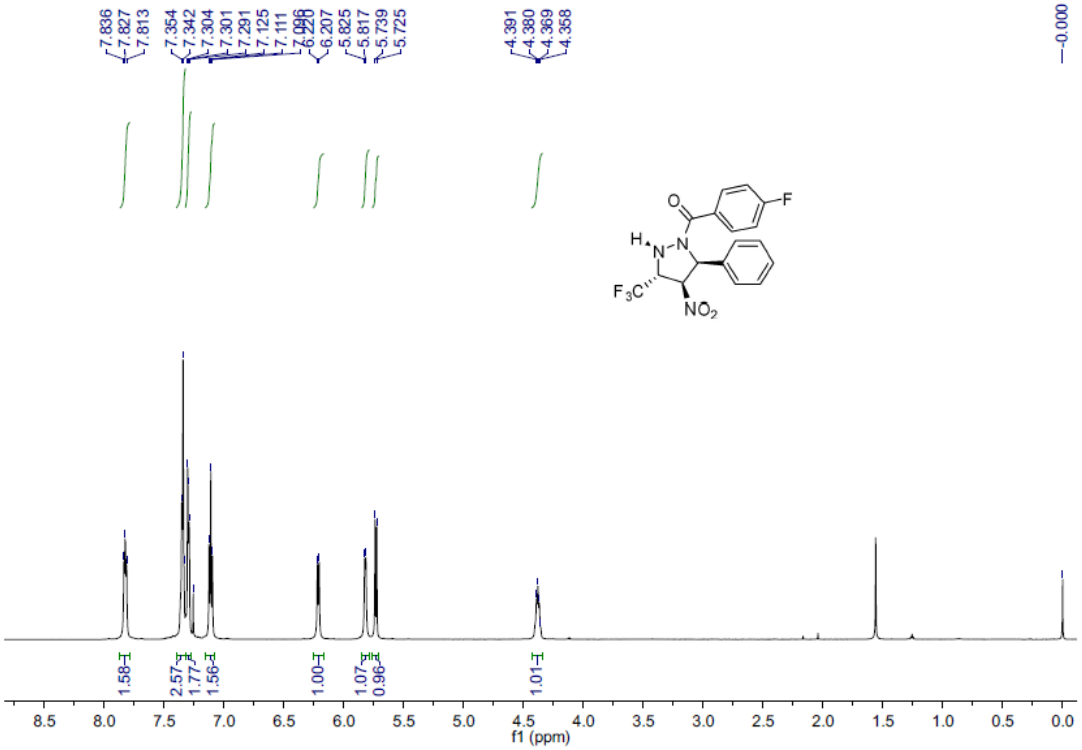
^{19}F NMR copies of compound **3da**:



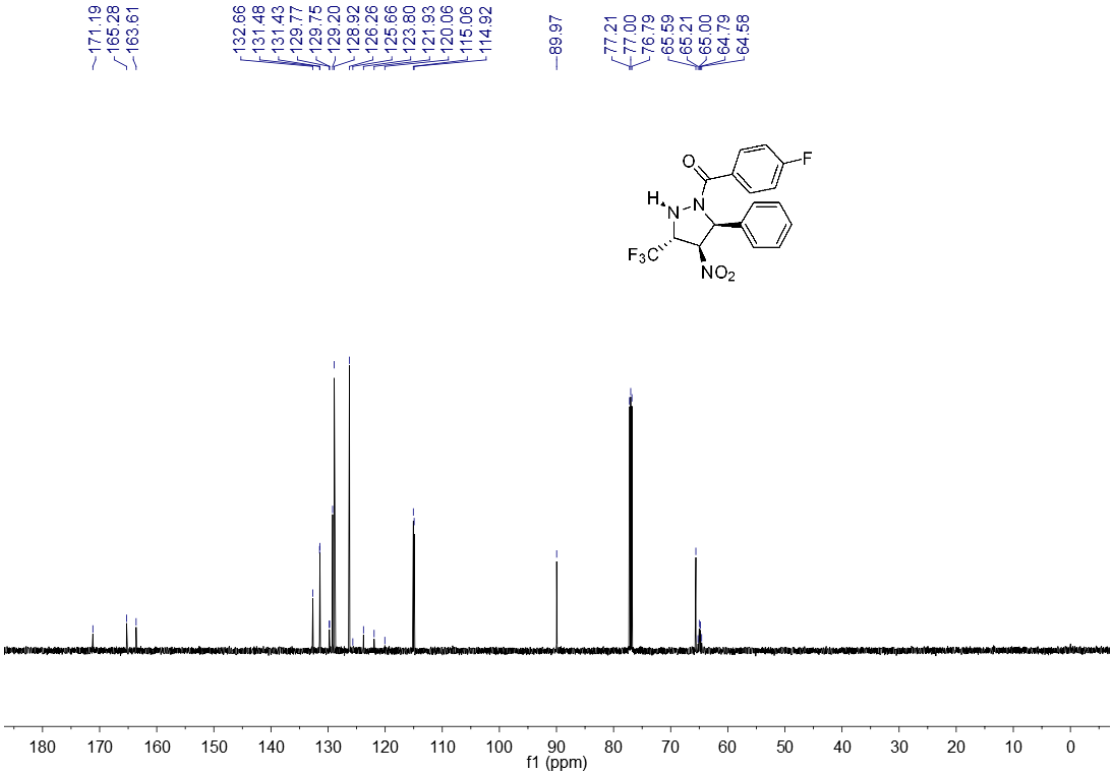
HRMS (ESI) of compound **3da**:



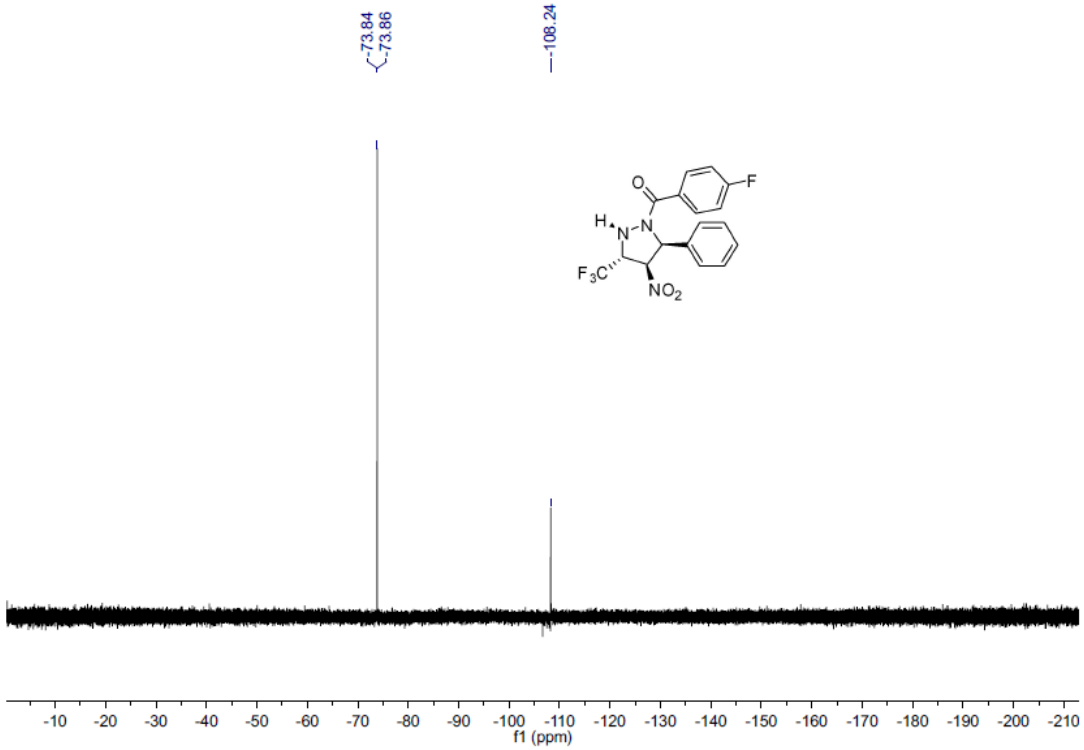
^{1}H NMR copies of compound **3ea**:



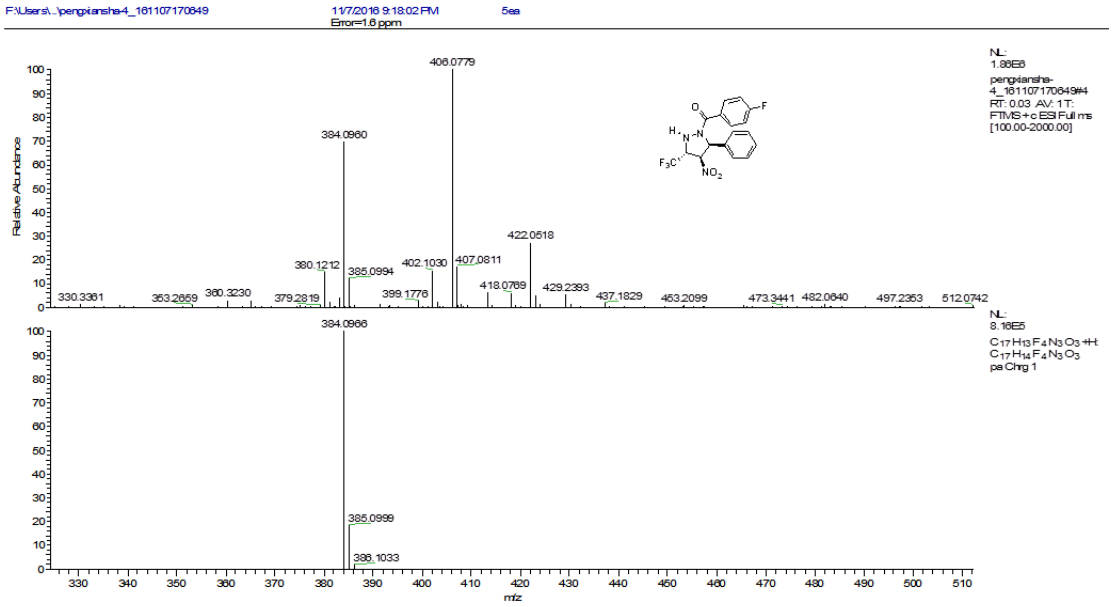
^{13}C NMR copies of compound **3ea**:



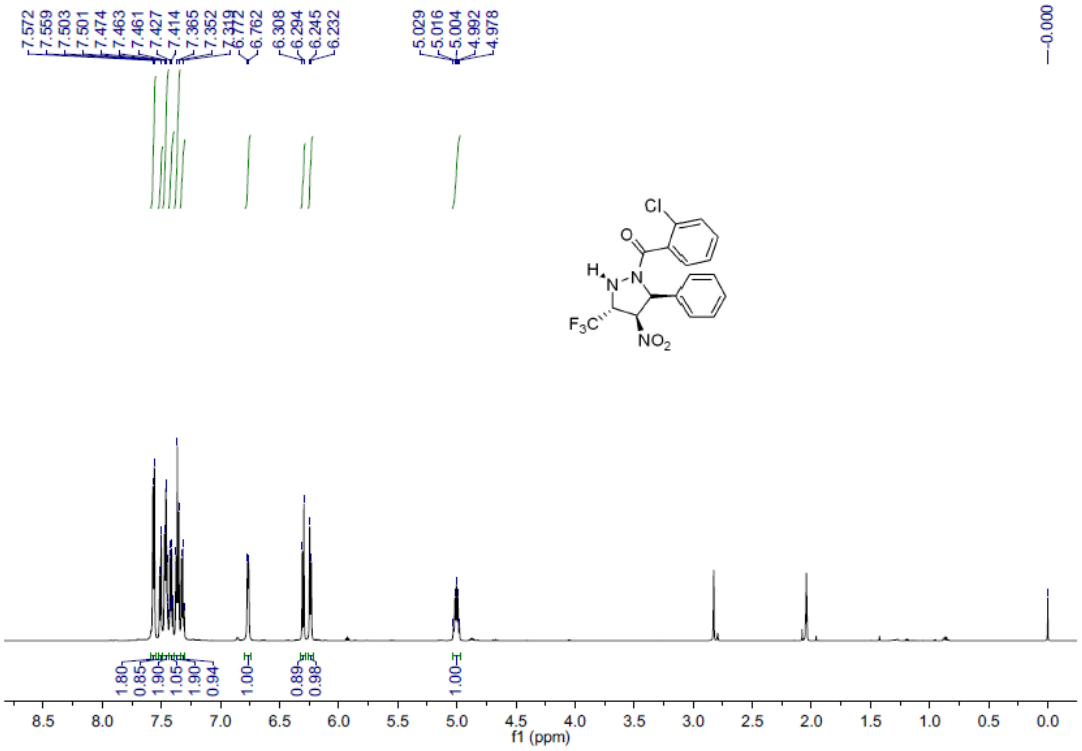
^{19}F NMR copies of compound **3ea**:



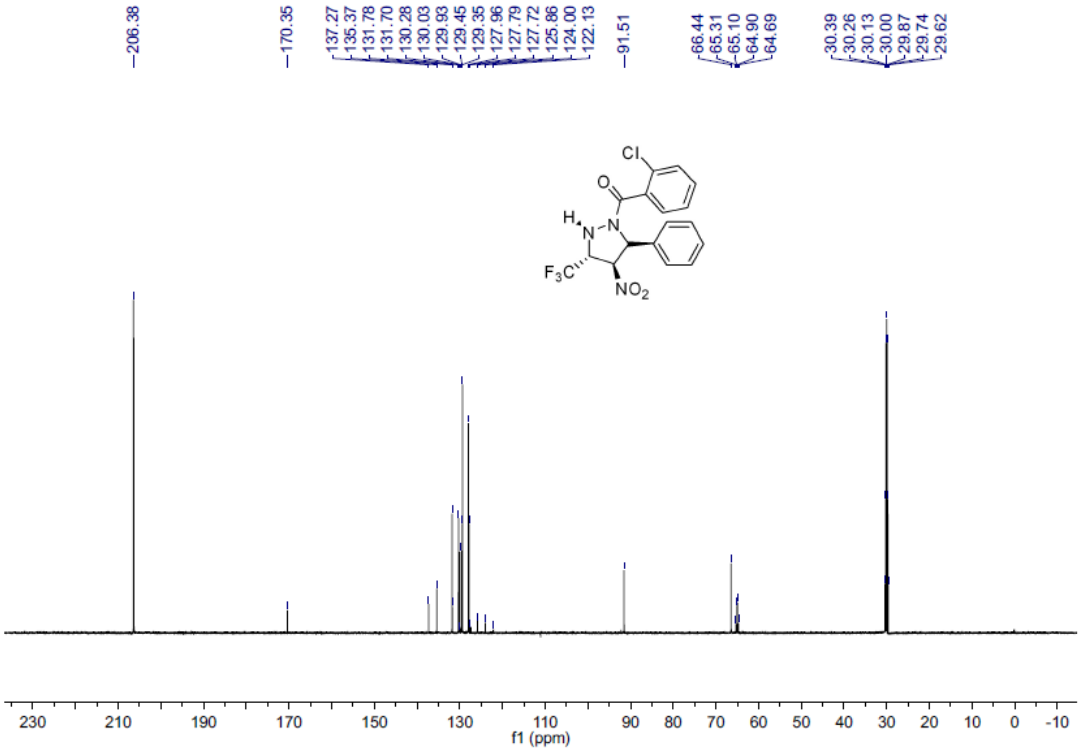
HRMS (ESI) of compound **3ea**:



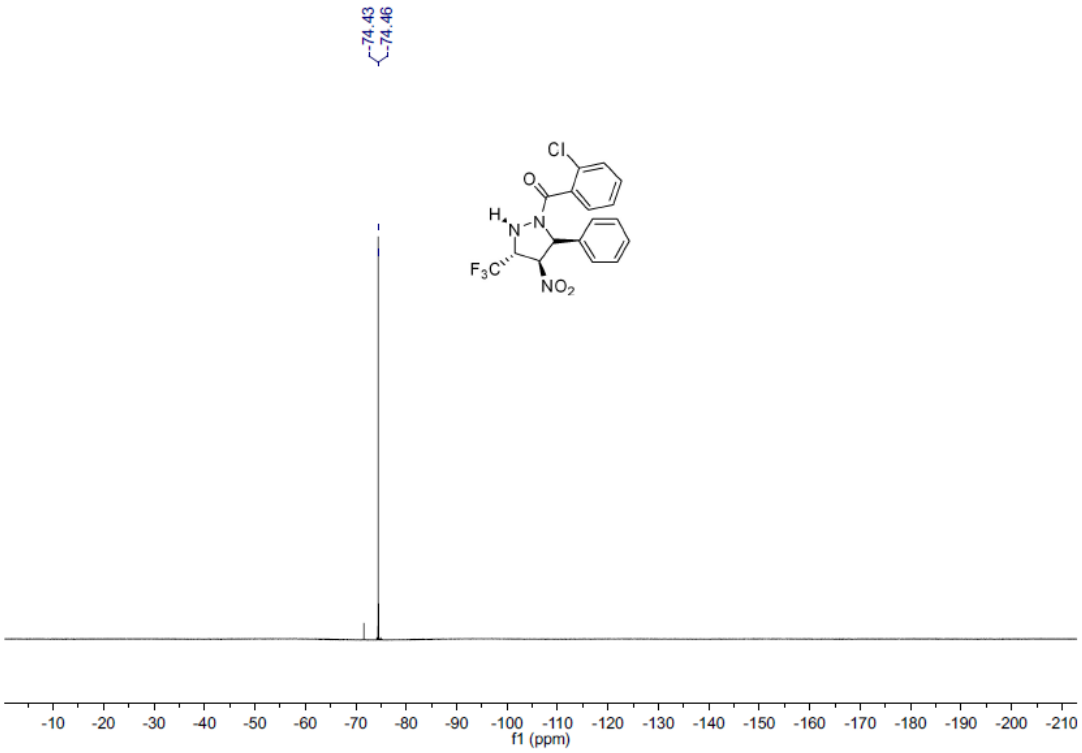
^{1}H NMR copies of compound **3fa**:



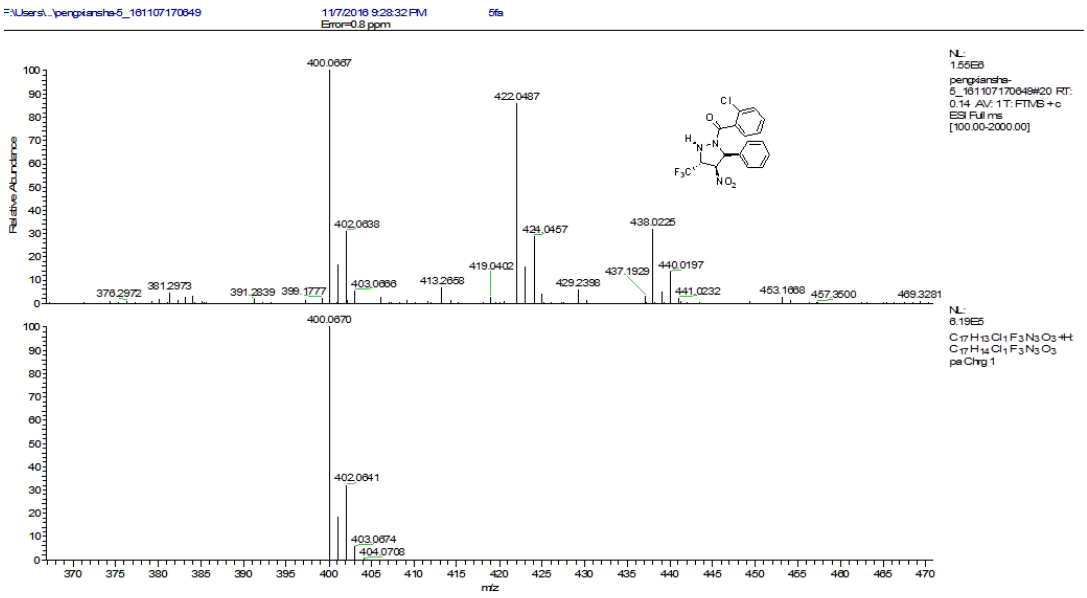
^{13}C NMR copies of compound **3fa**:



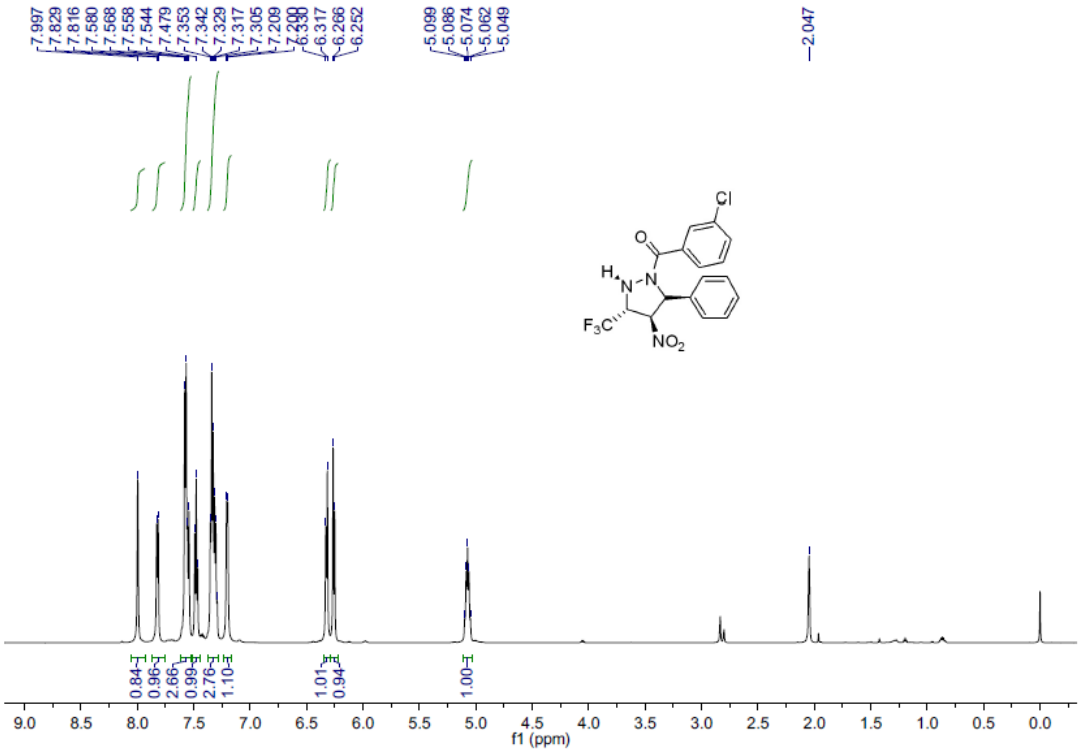
^{19}F NMR copies of compound **3fa**:



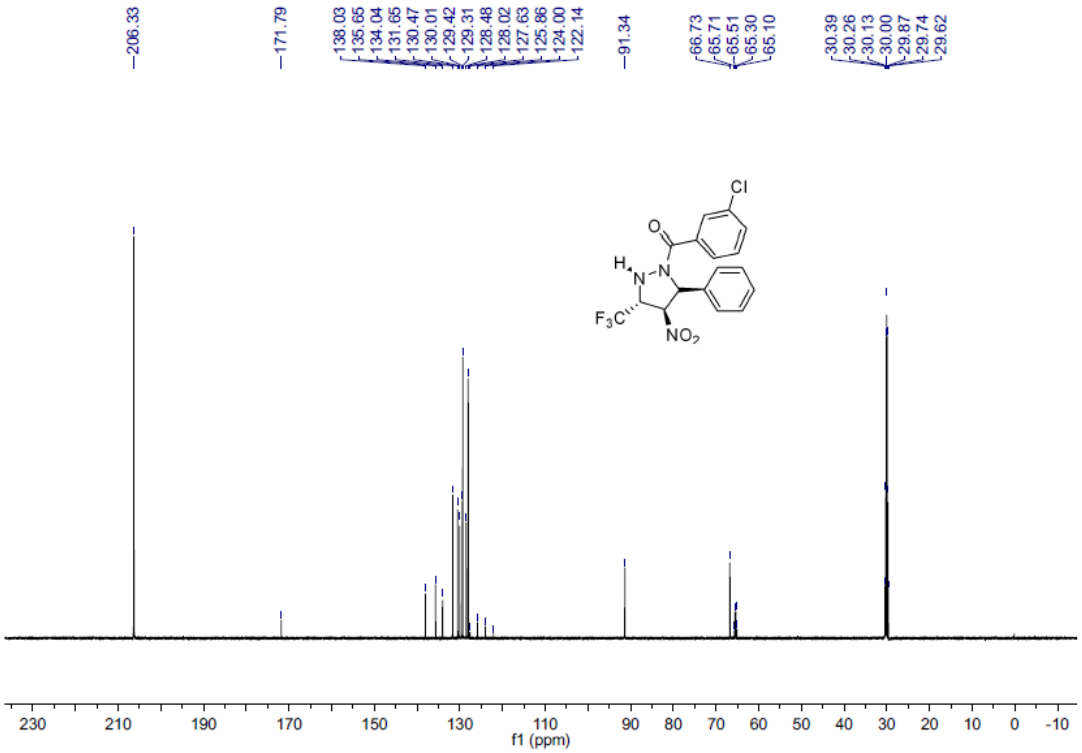
HRMS (ESI) of compound **3fa**:



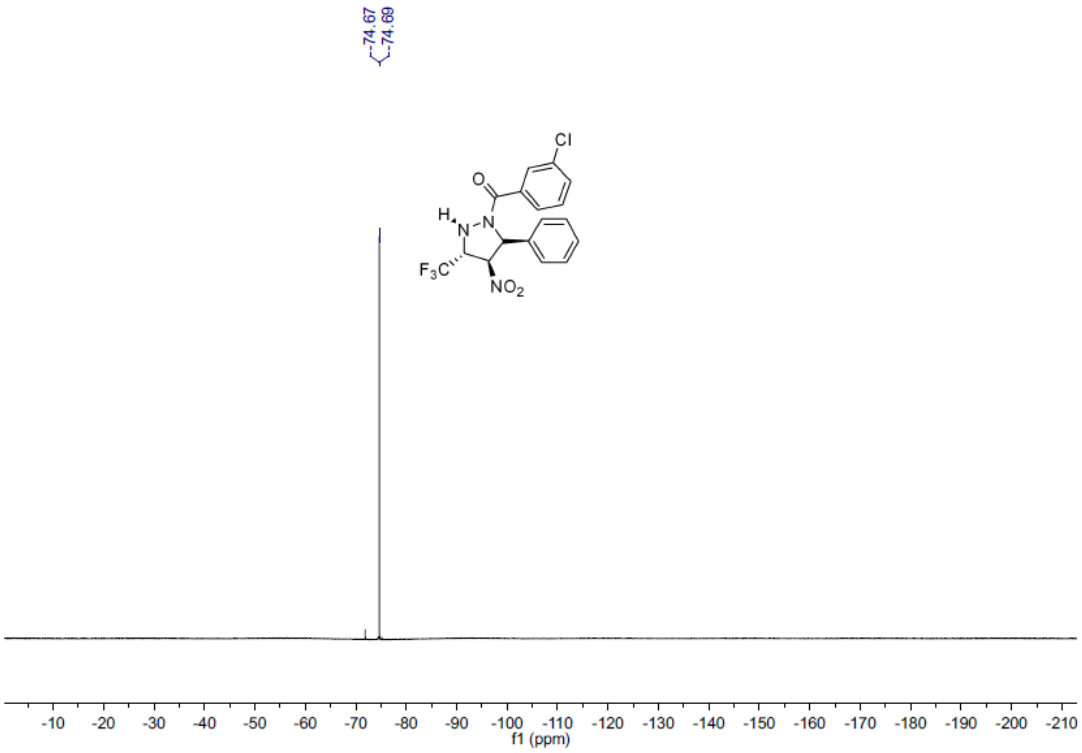
^{1}H NMR copies of compound **3ga**:



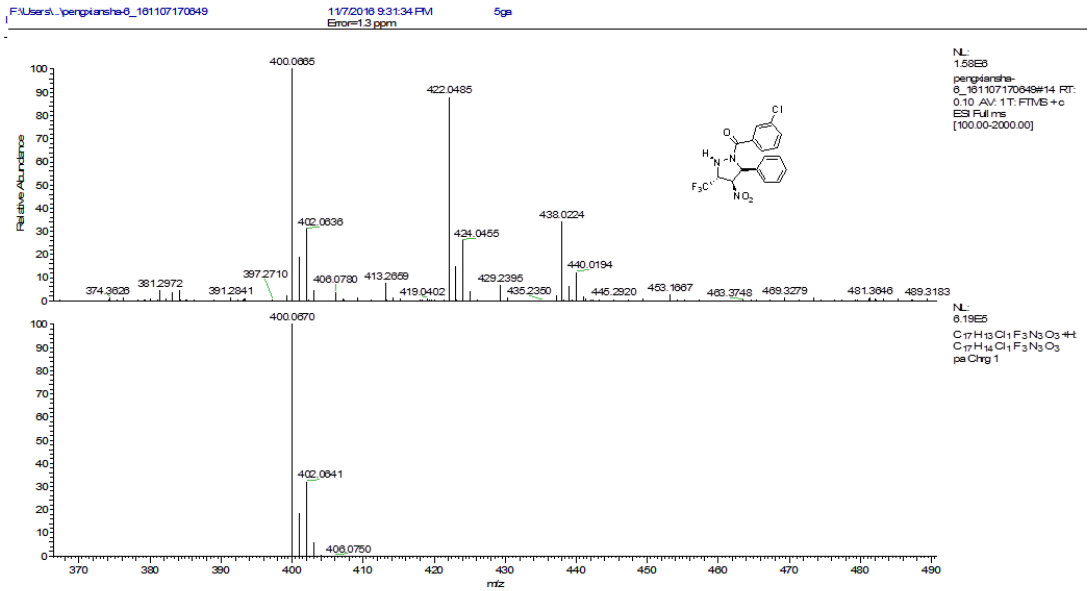
^{13}C NMR copies of compound **3ga**:



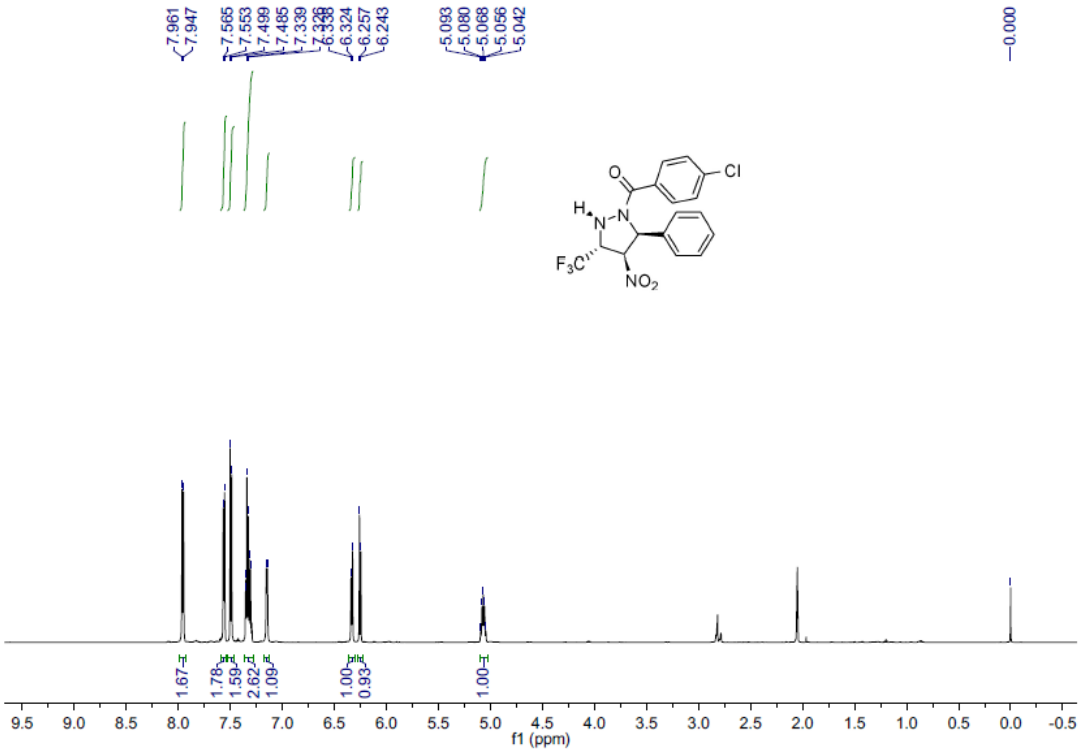
^{19}F NMR copies of compound **3ga**:



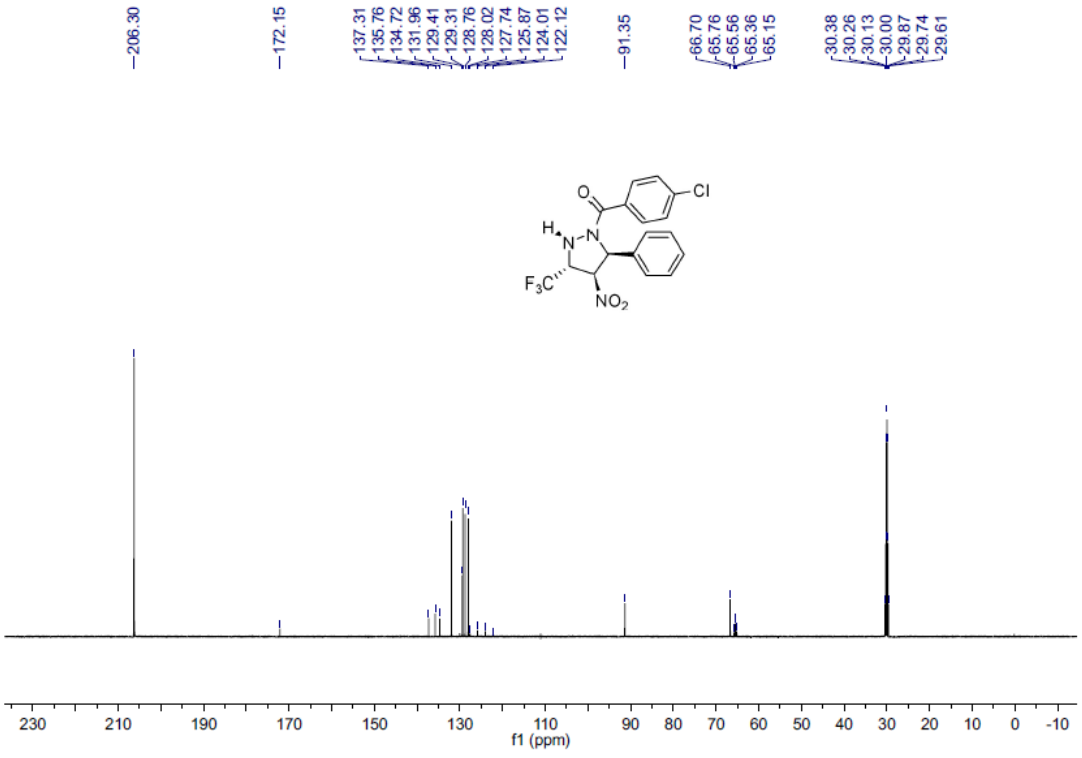
HRMS (ESI) of compound **3ga**:



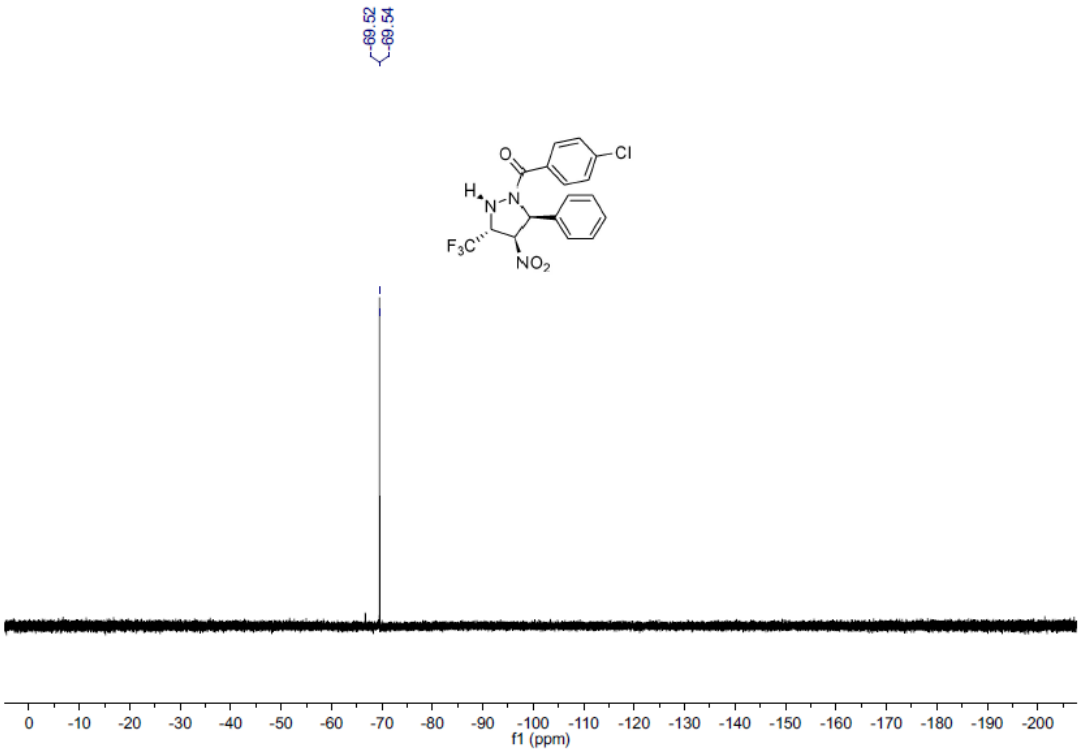
^{1}H NMR copies of compound **3ha**:



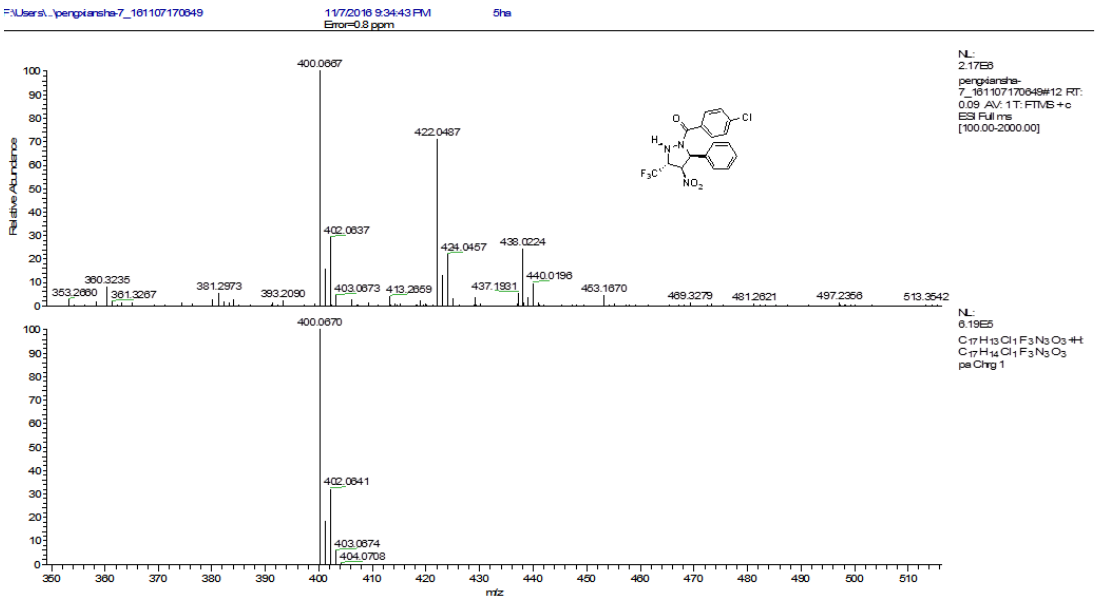
^{13}C NMR copies of compound **3ha**:



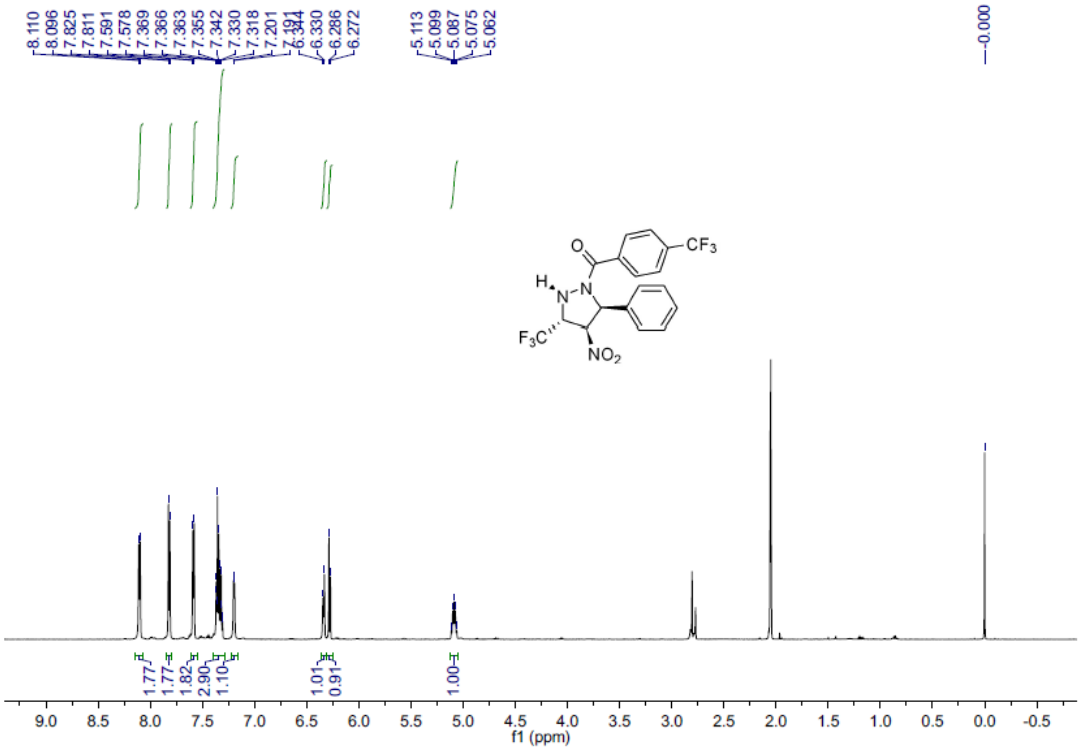
^{19}F NMR copies of compound **3ha**:



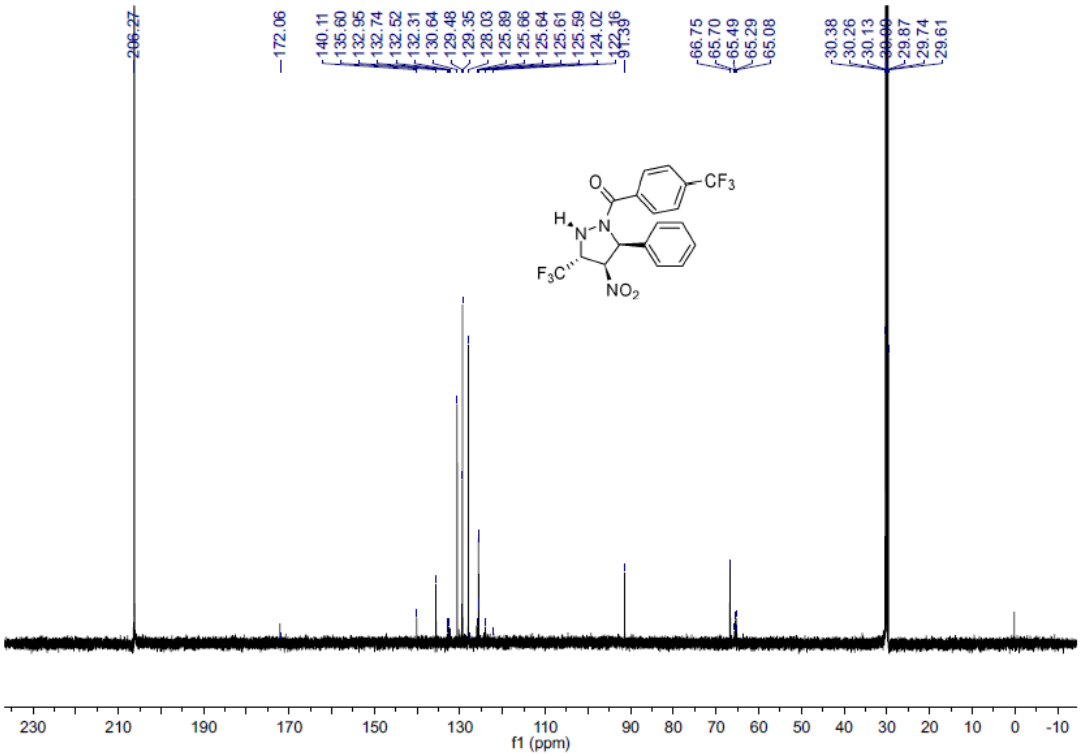
HRMS (ESI) of compound **3ha**:



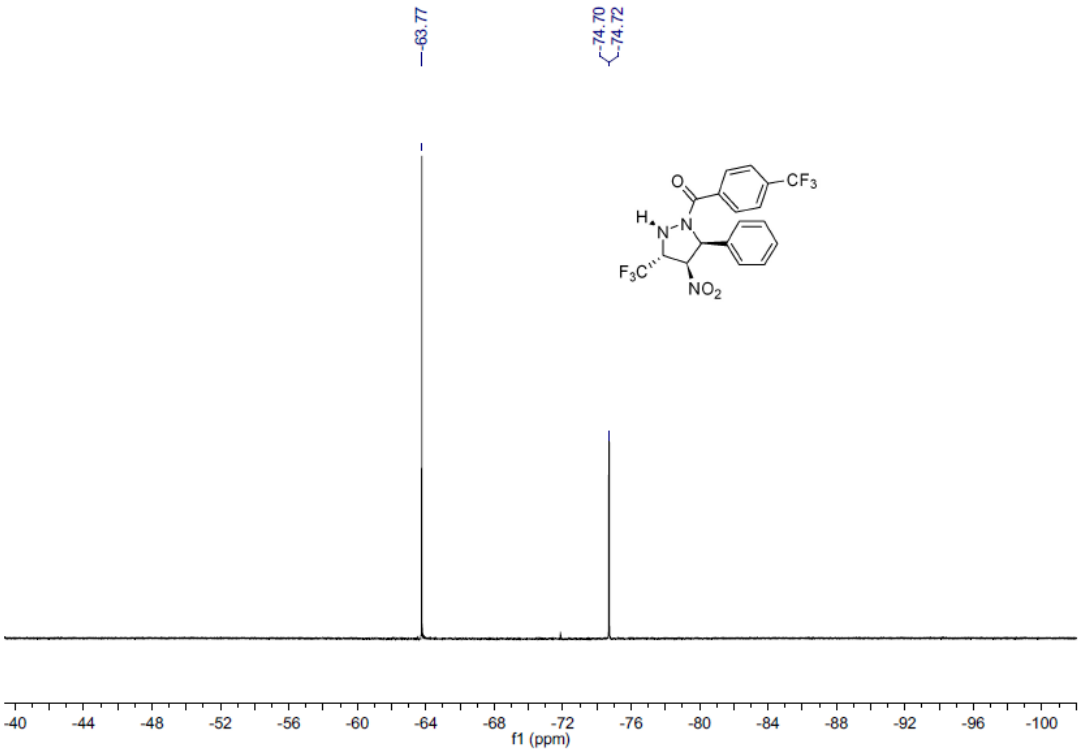
^{1}H NMR copies of compound **3ia**:



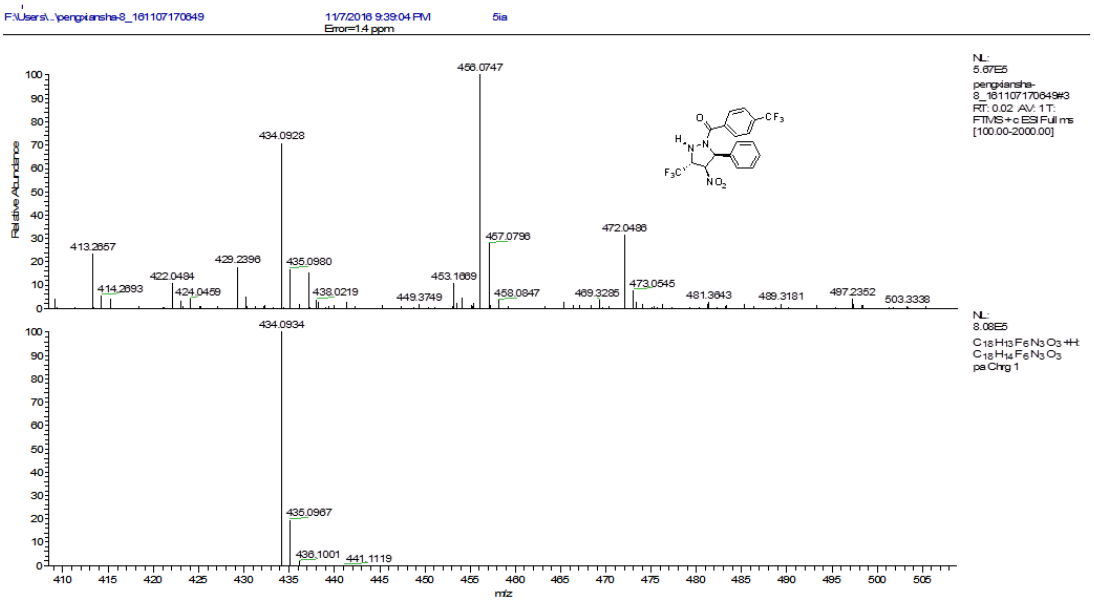
^{13}C NMR copies of compound **3ia**:



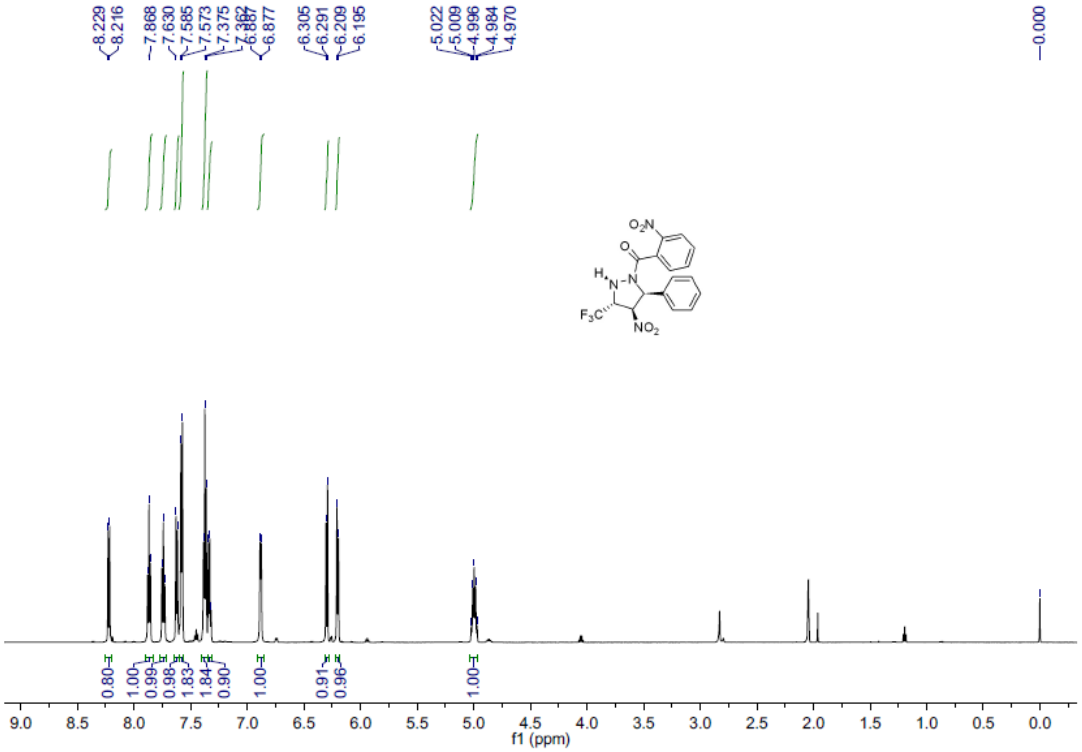
^{19}F NMR copies of compound **3ia**:



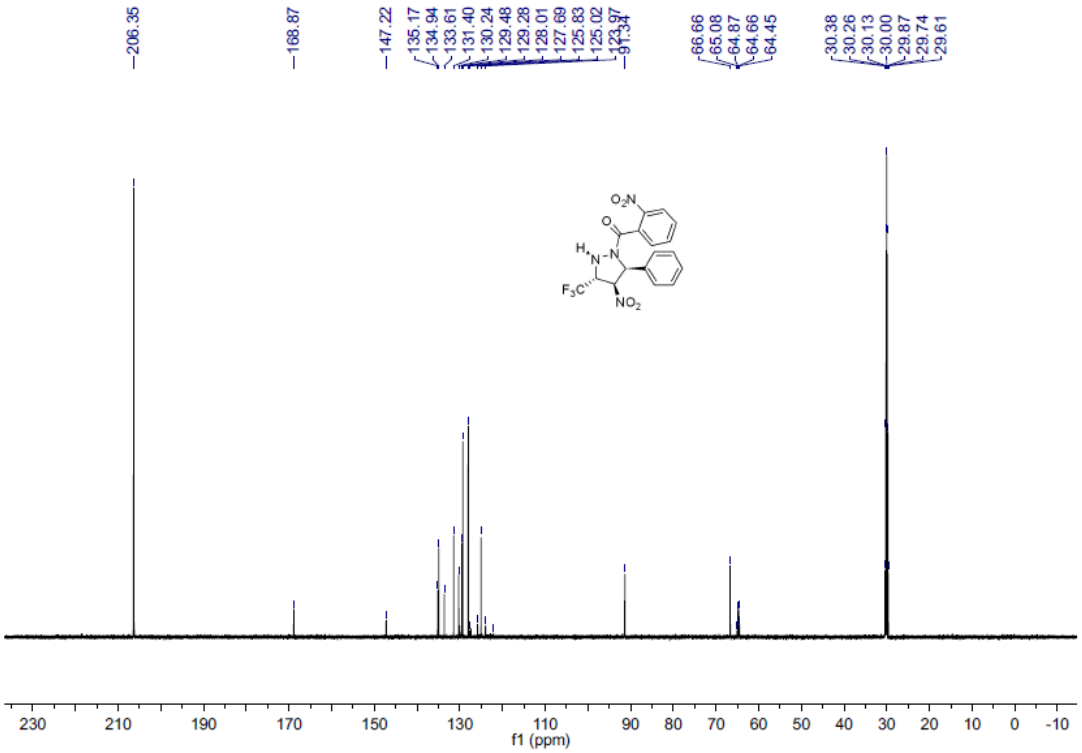
HRMS (ESI) of compound **3ia**:



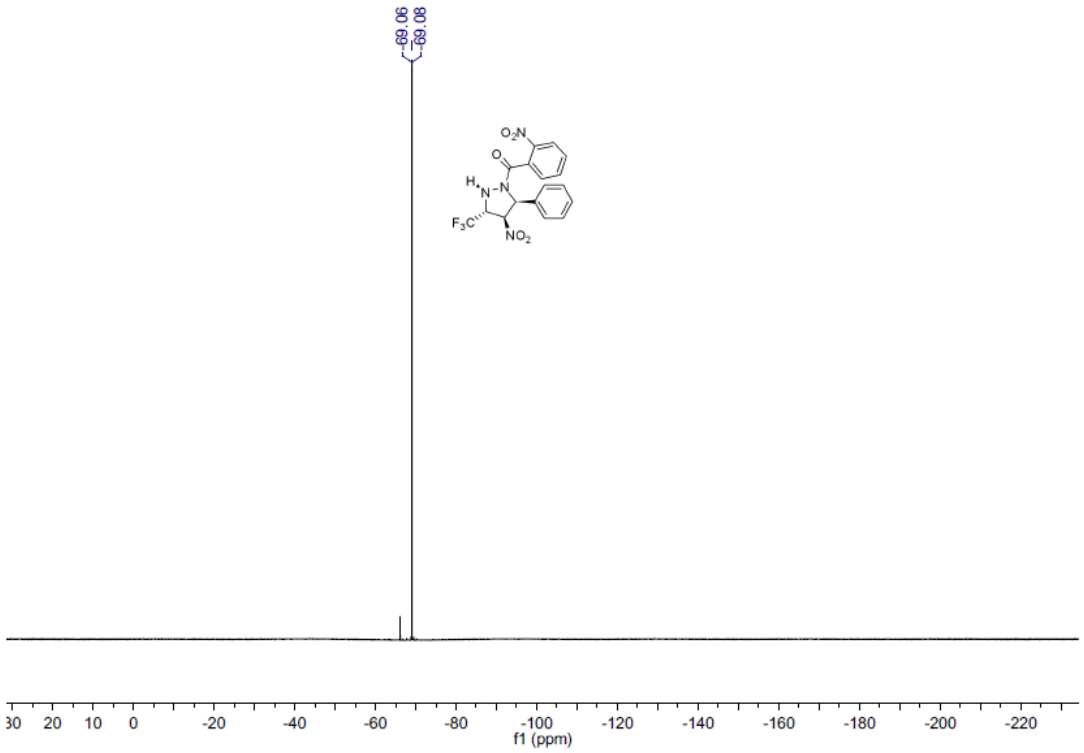
^{1}H NMR copies of compound **3ja**:



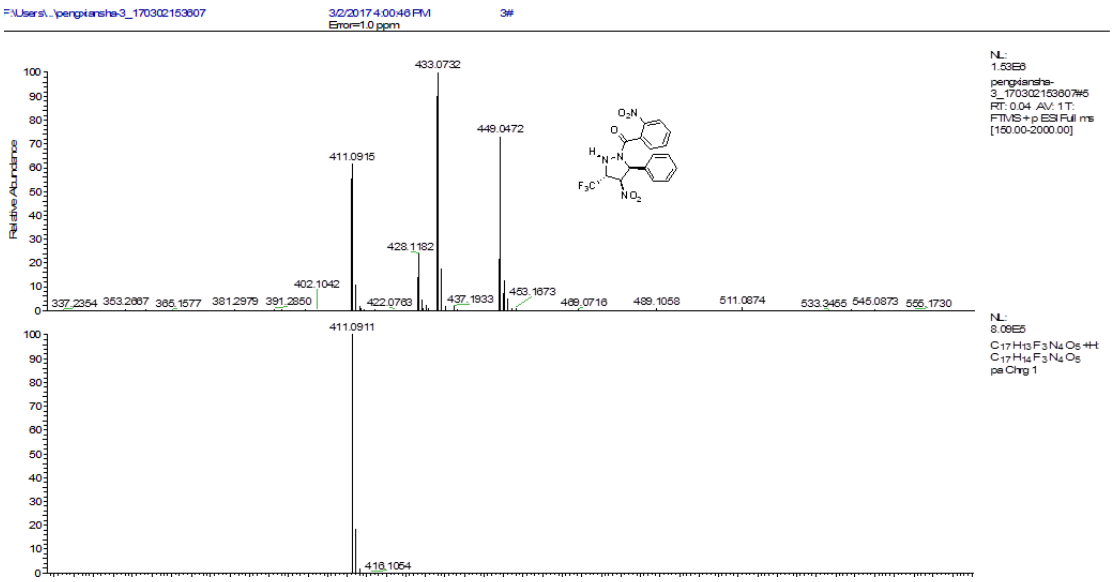
^{13}C NMR copies of compound **3ja**:



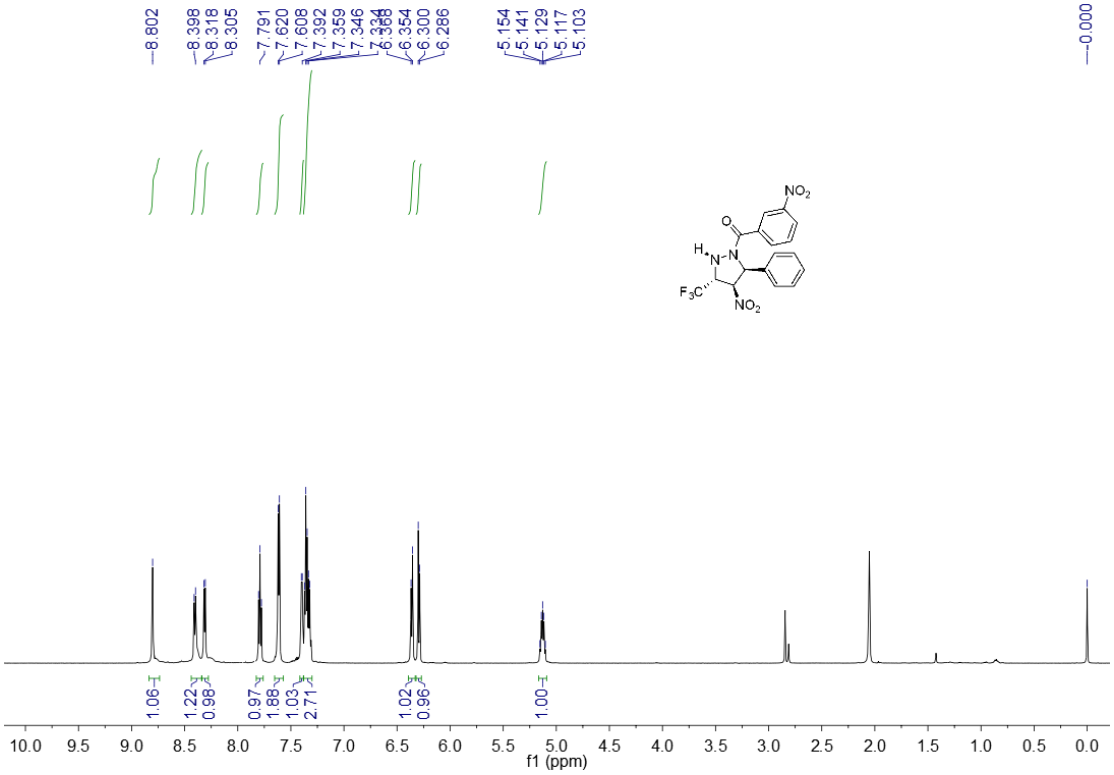
^{1}F NMR copies of compound **3ja**:



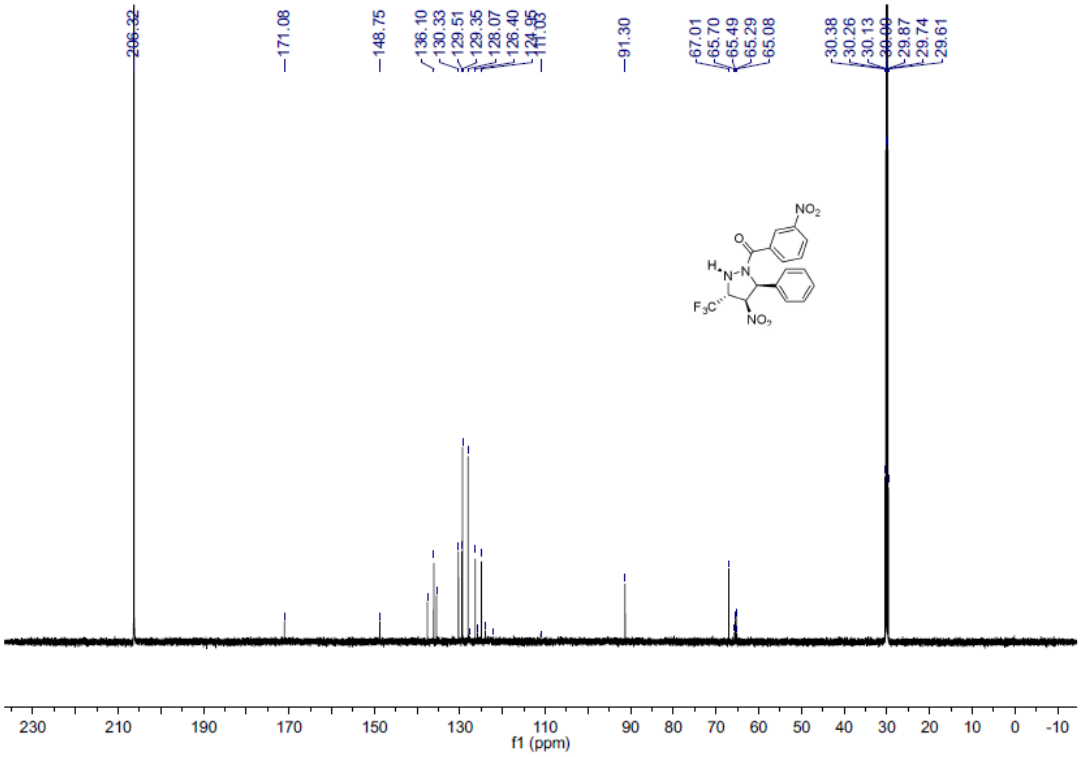
HRMS (ESI) of compound **3ja**:



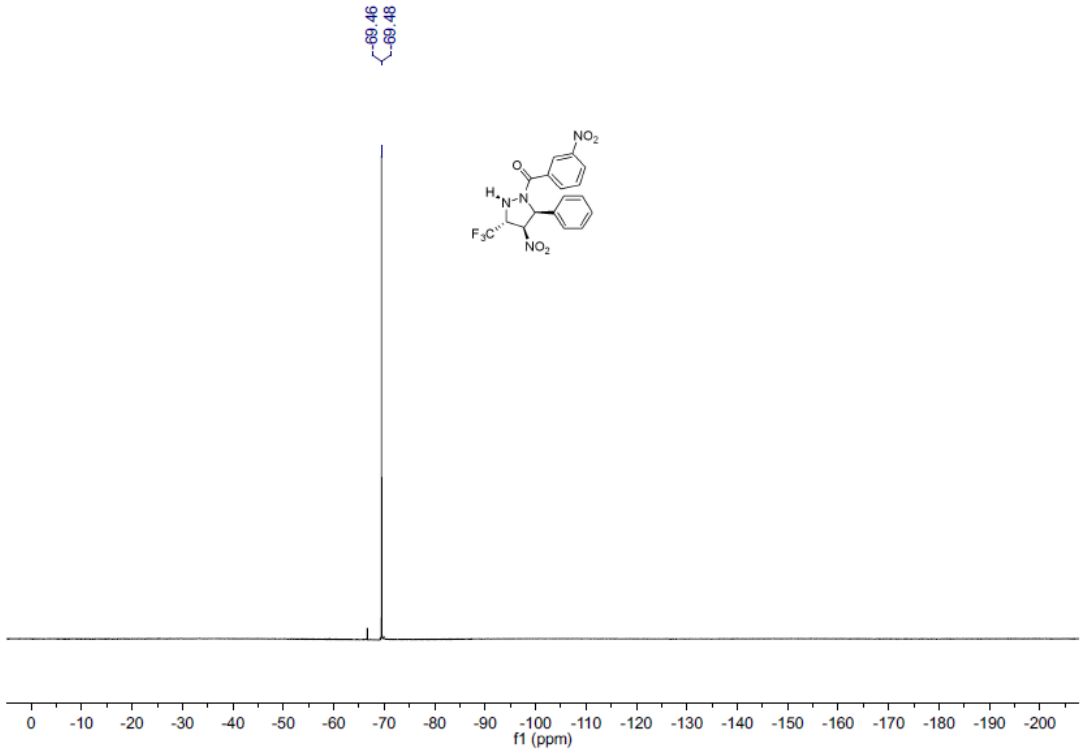
^{1}H NMR copies of compound **3ka**:



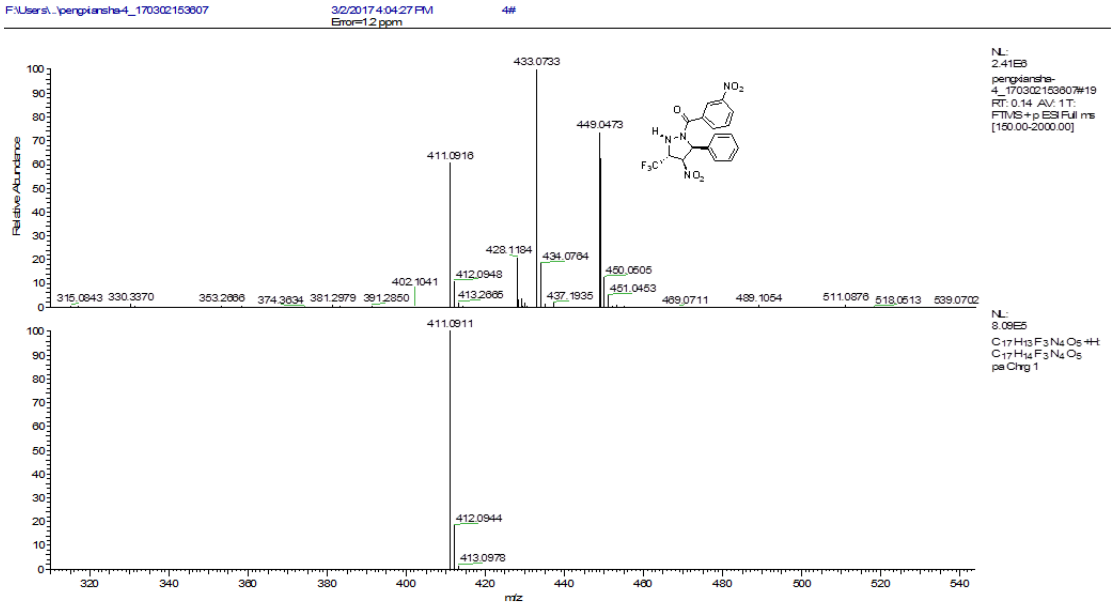
^{13}C NMR copies of compound **3ka**:



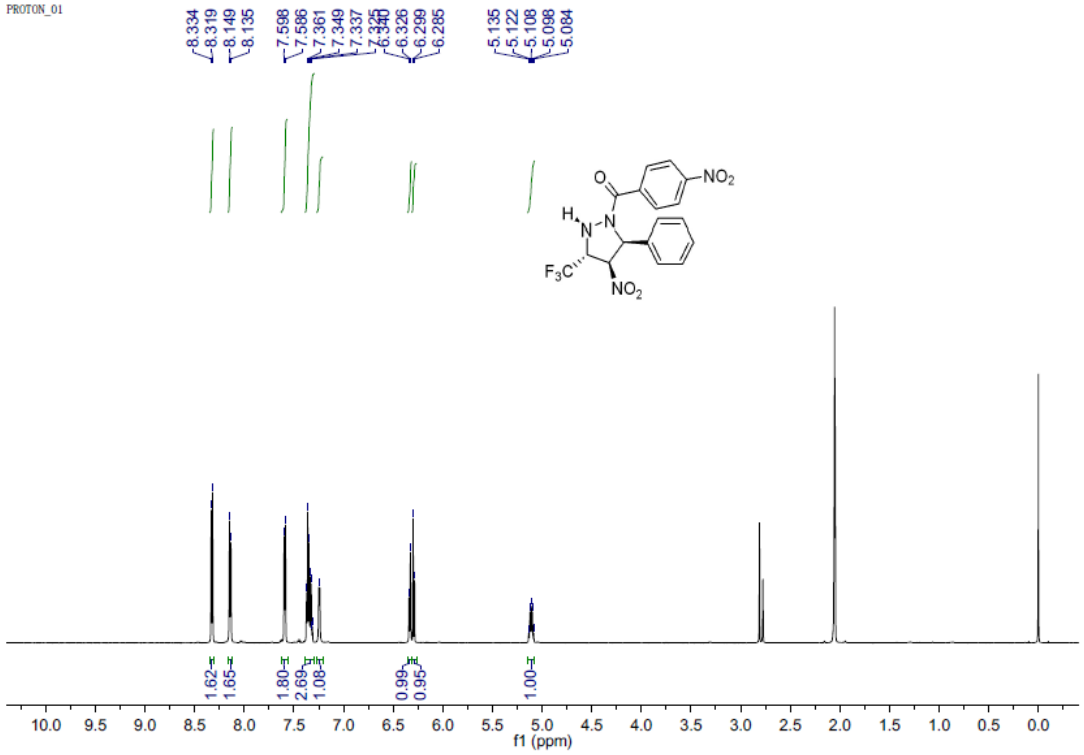
^{19}F NMR copies of compound **3ka**:



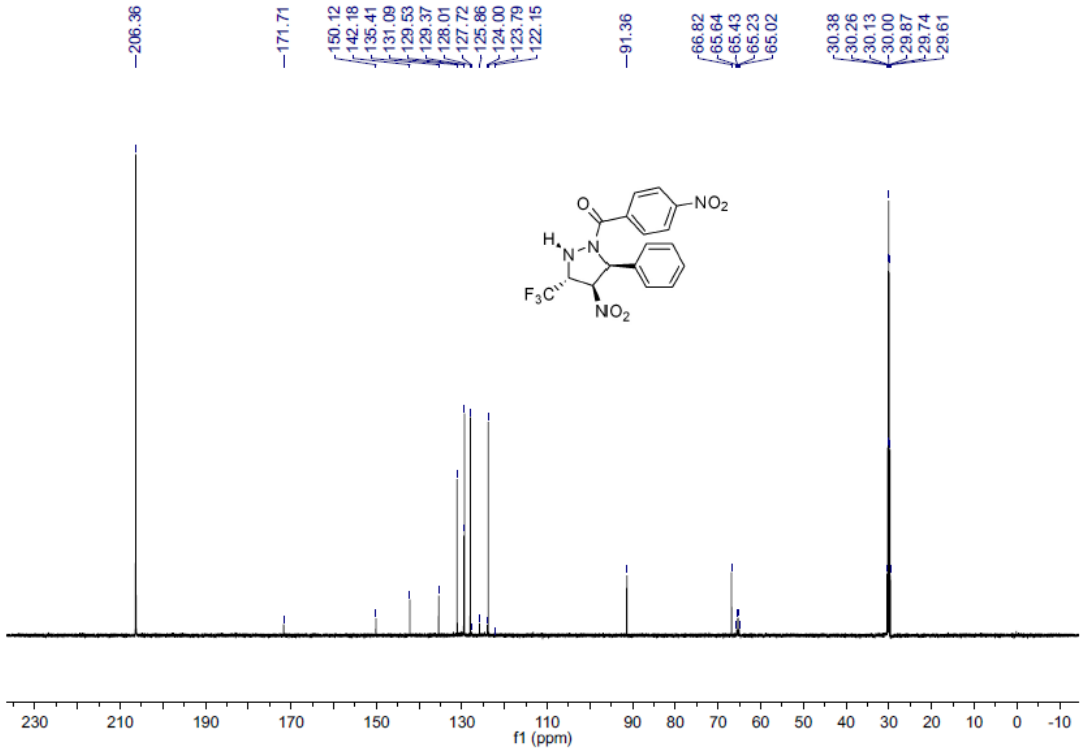
HRMS (ESI) of compound **3ka**:



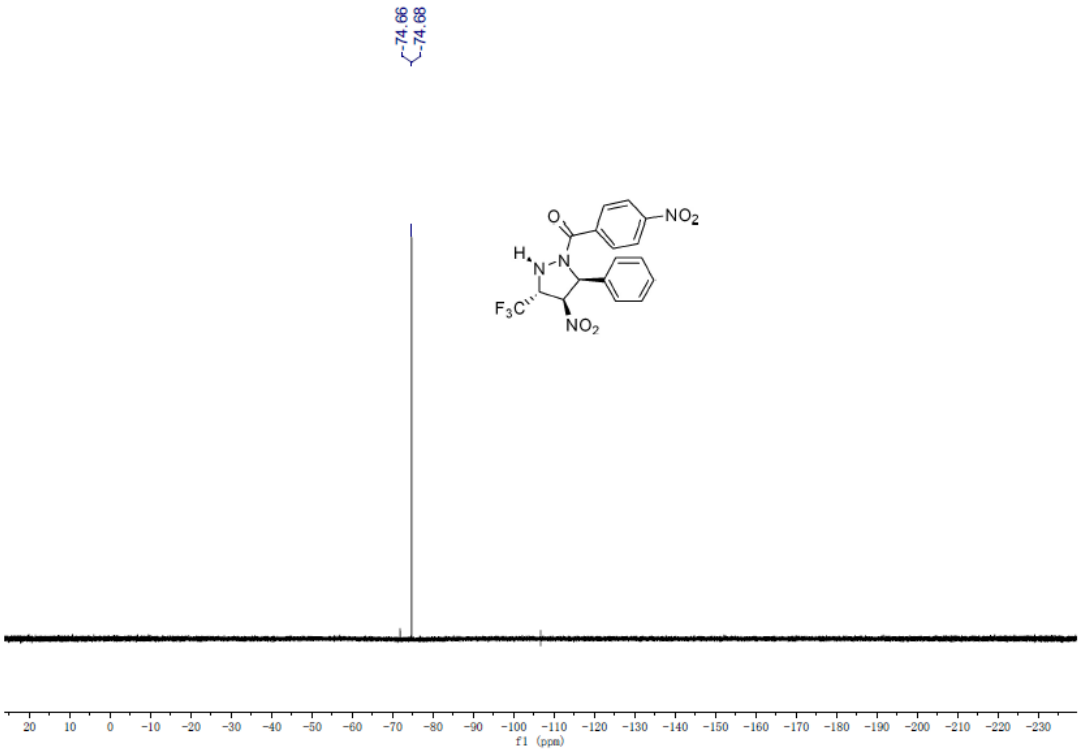
^{1}H NMR copies of compound **3la**:



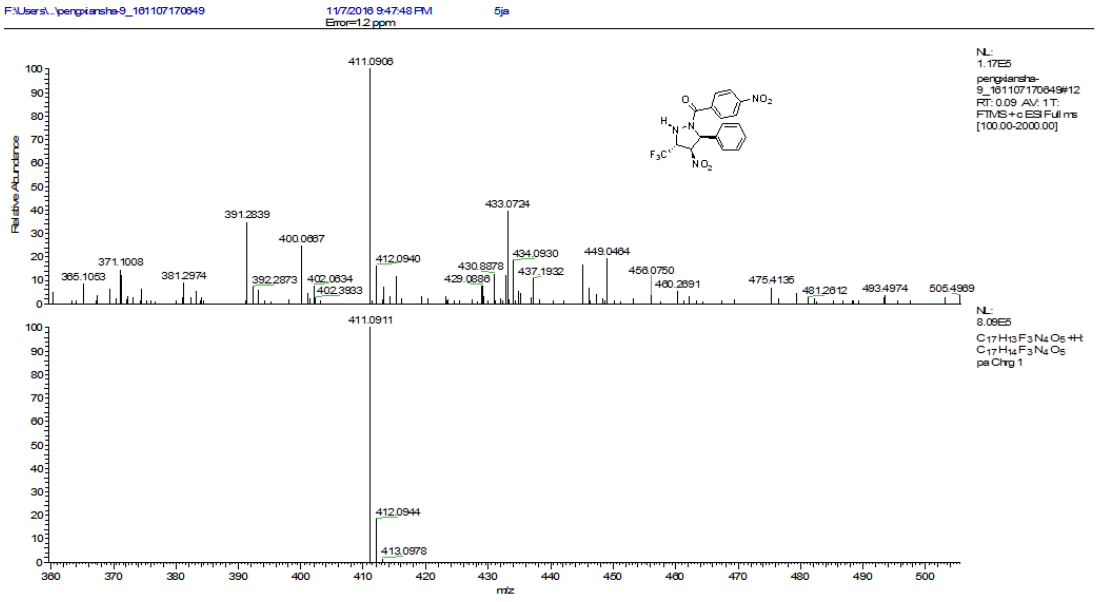
^{13}C NMR copies of compound **3la**:



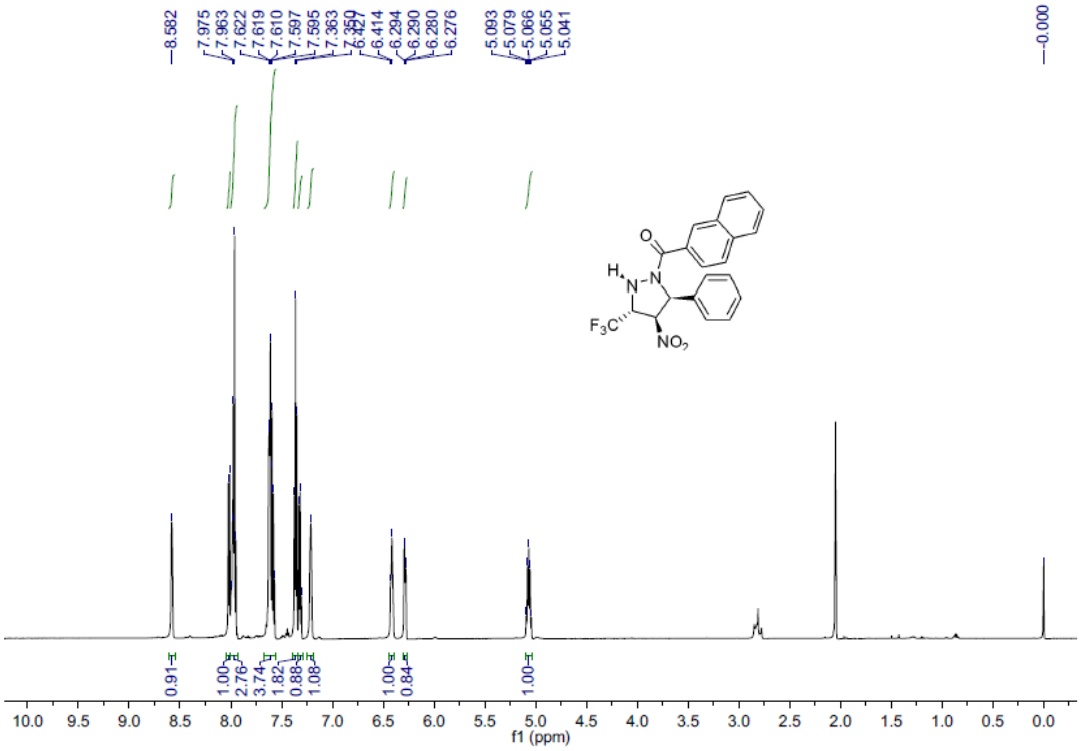
^{19}F NMR copies of compound **3la**:



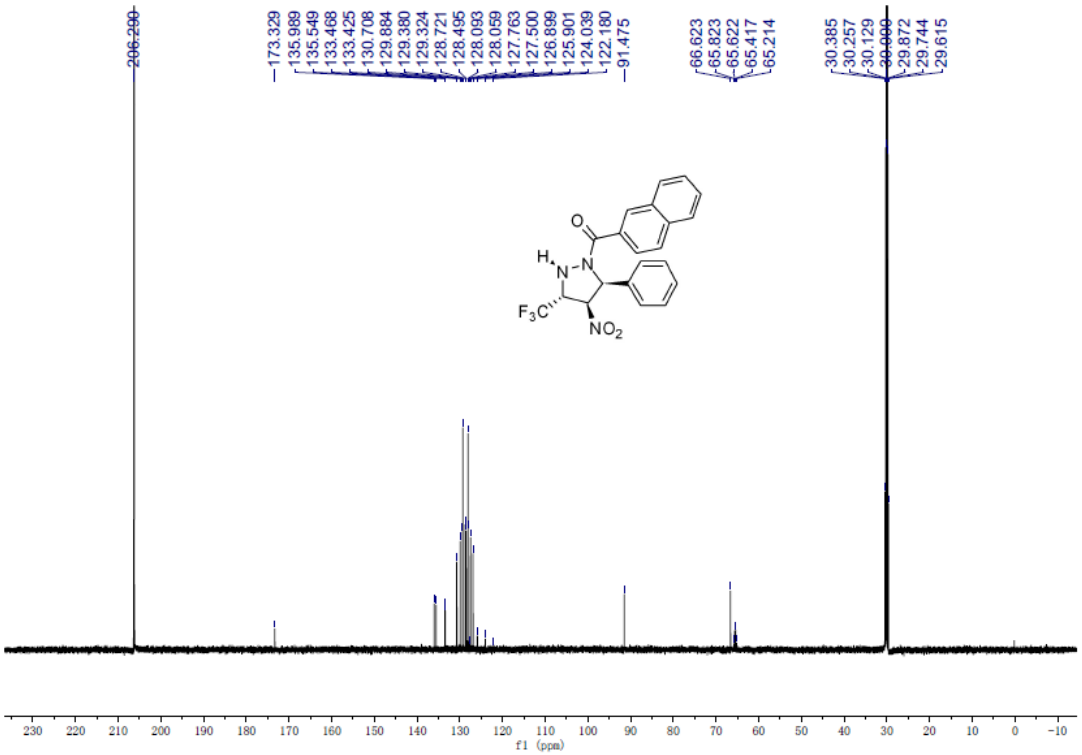
HRMS (ESI) of compound **3la**:



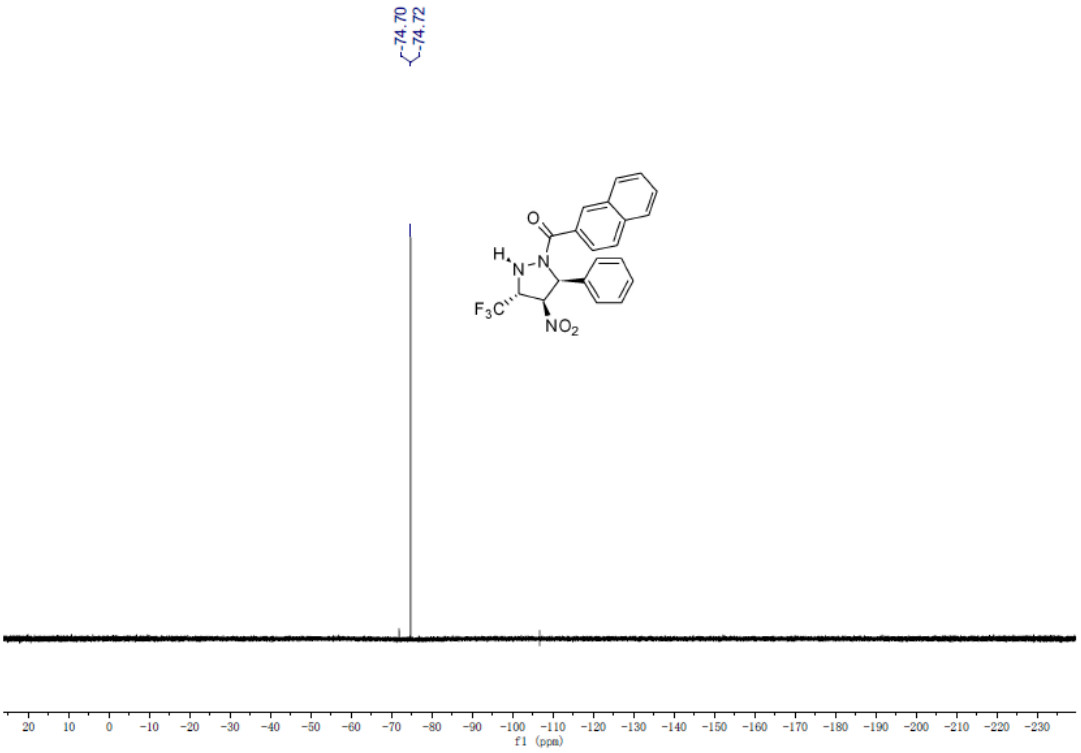
^{1}H NMR copies of compound **3ma**:



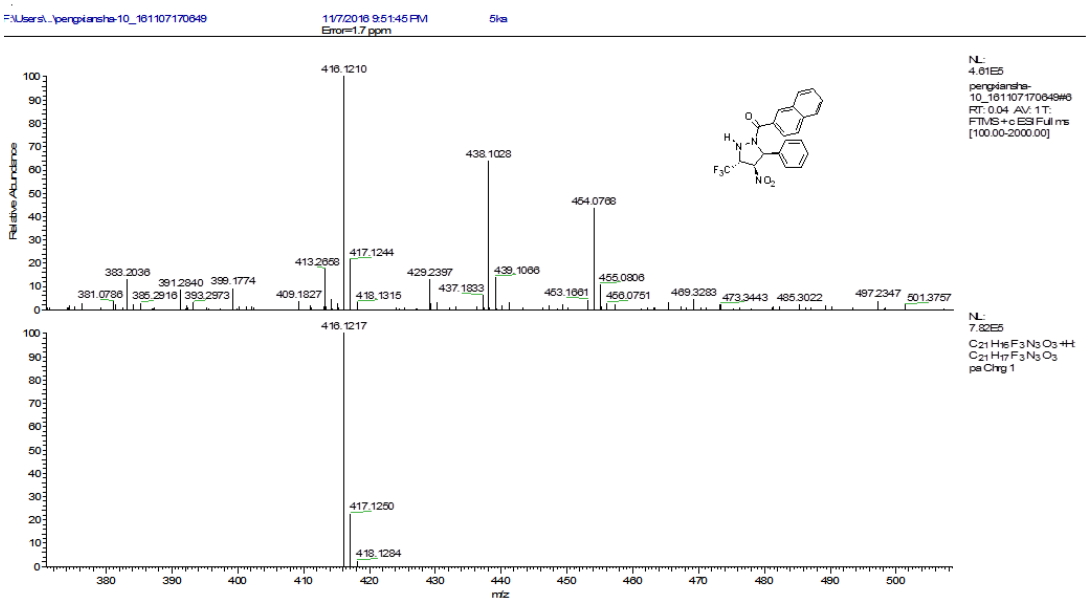
^{13}C NMR copies of compound **3ma**:



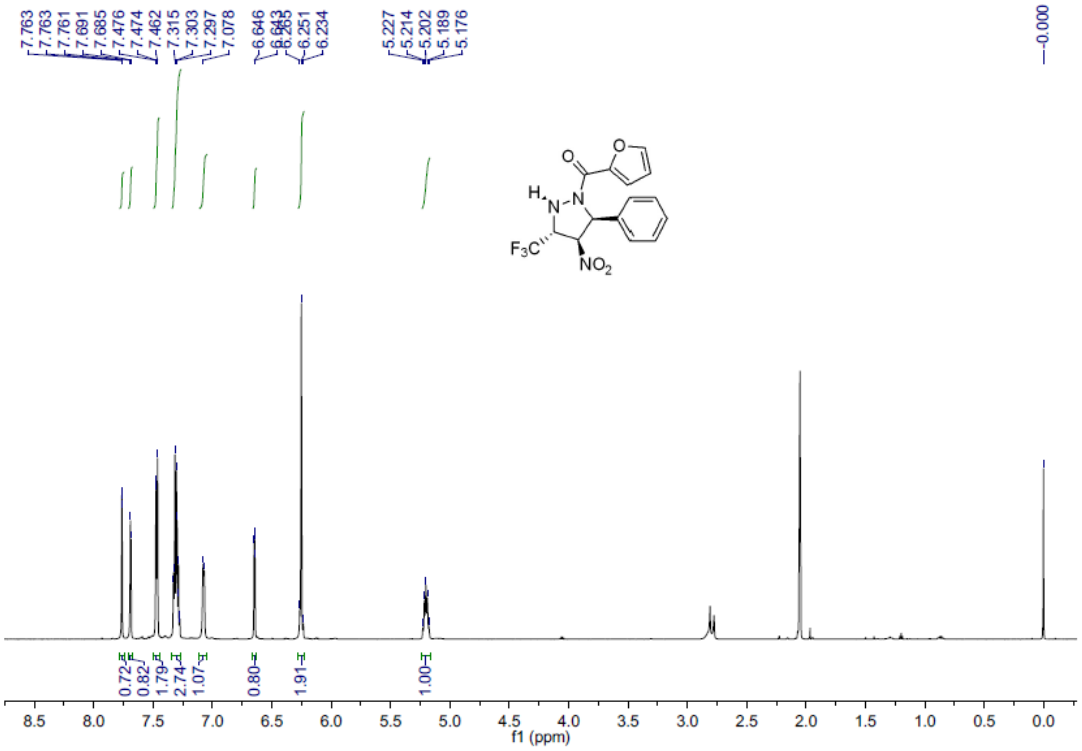
^{19}F NMR copies of compound **3ma**:



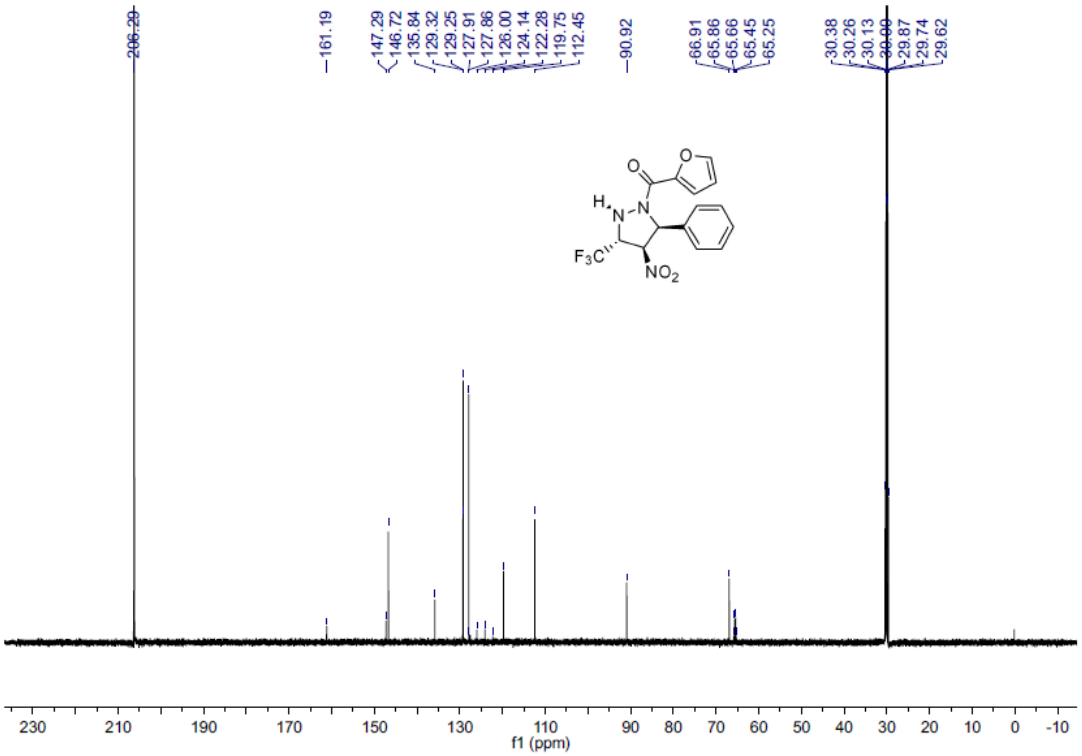
HRMS (ESI) of compound **3ma**:



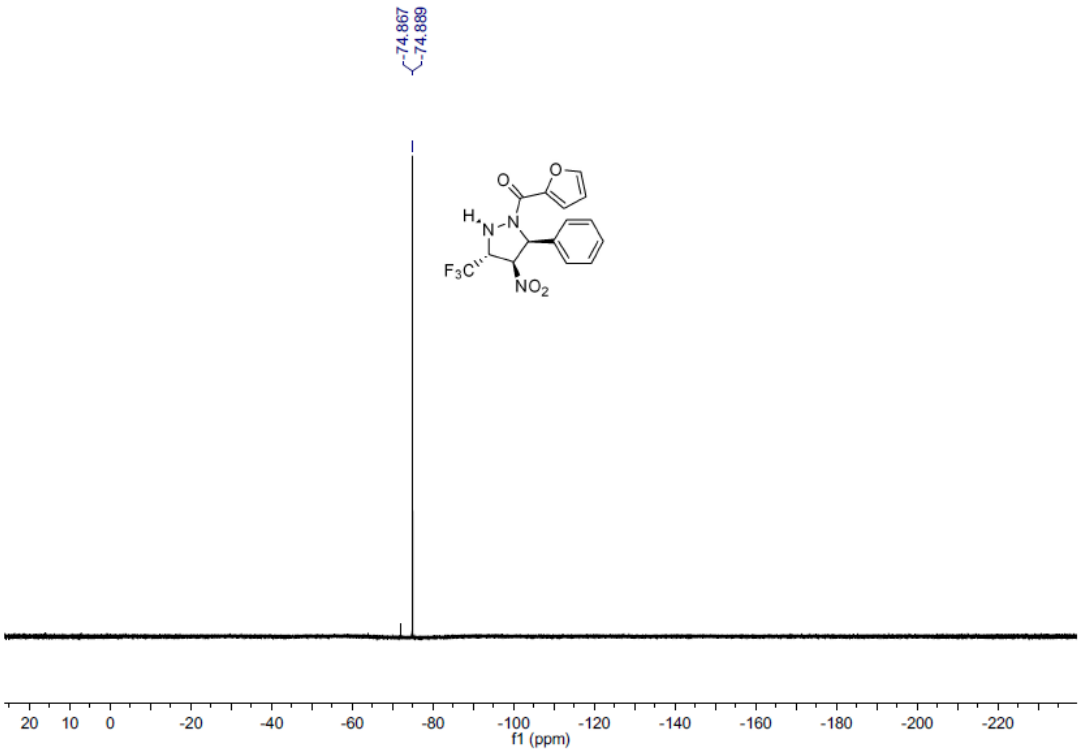
^{1}H NMR copies of compound **3na**:



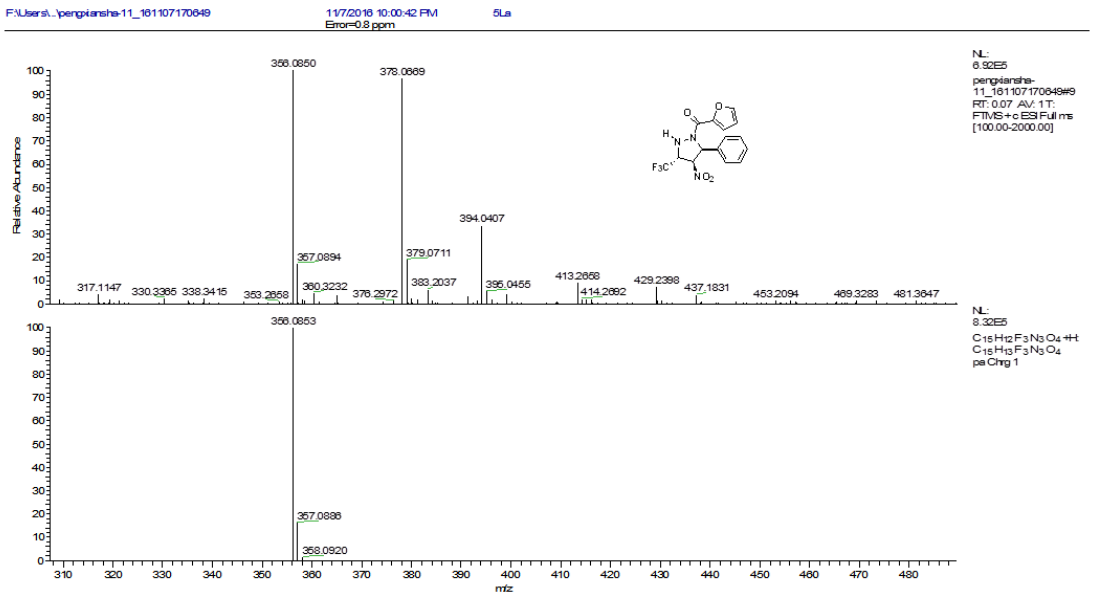
^{13}C NMR copies of compound **3na**:



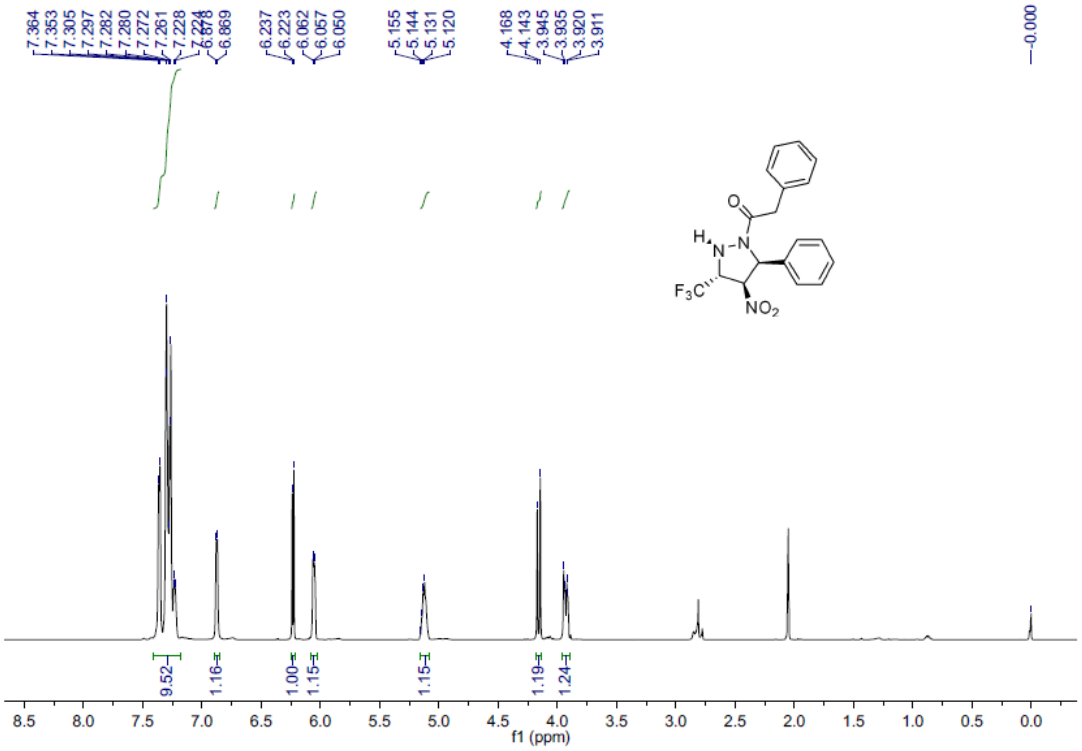
^{19}F NMR copies of compound **3na**:



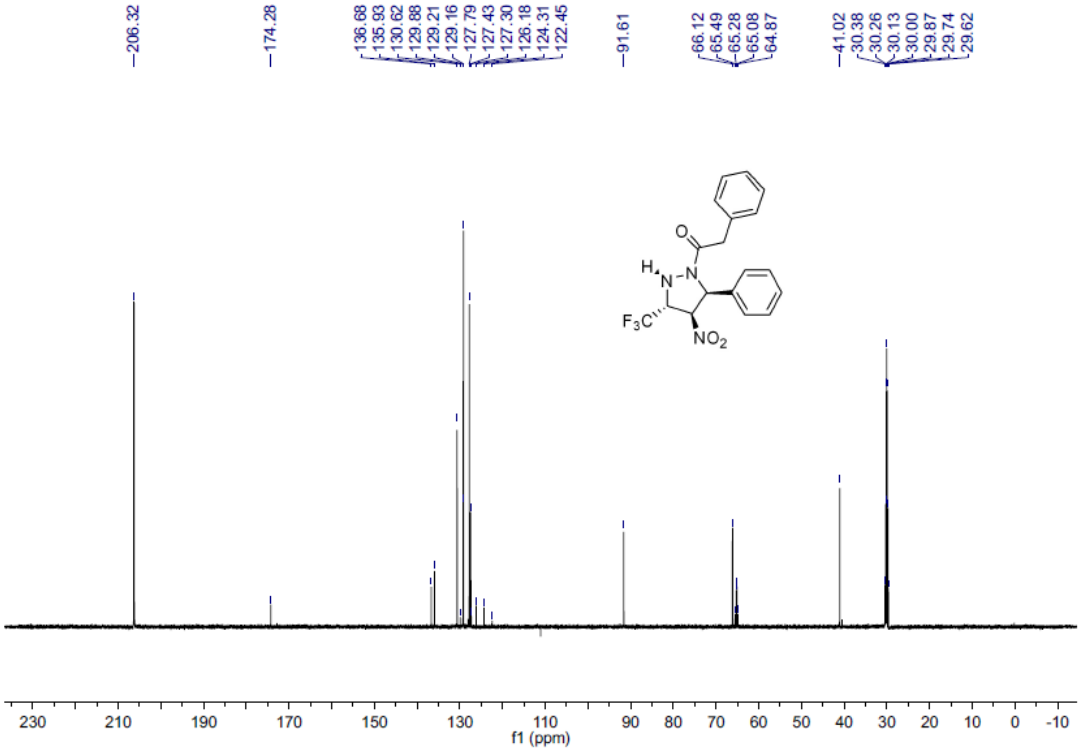
HRMS (ESI) of compound **3na**:



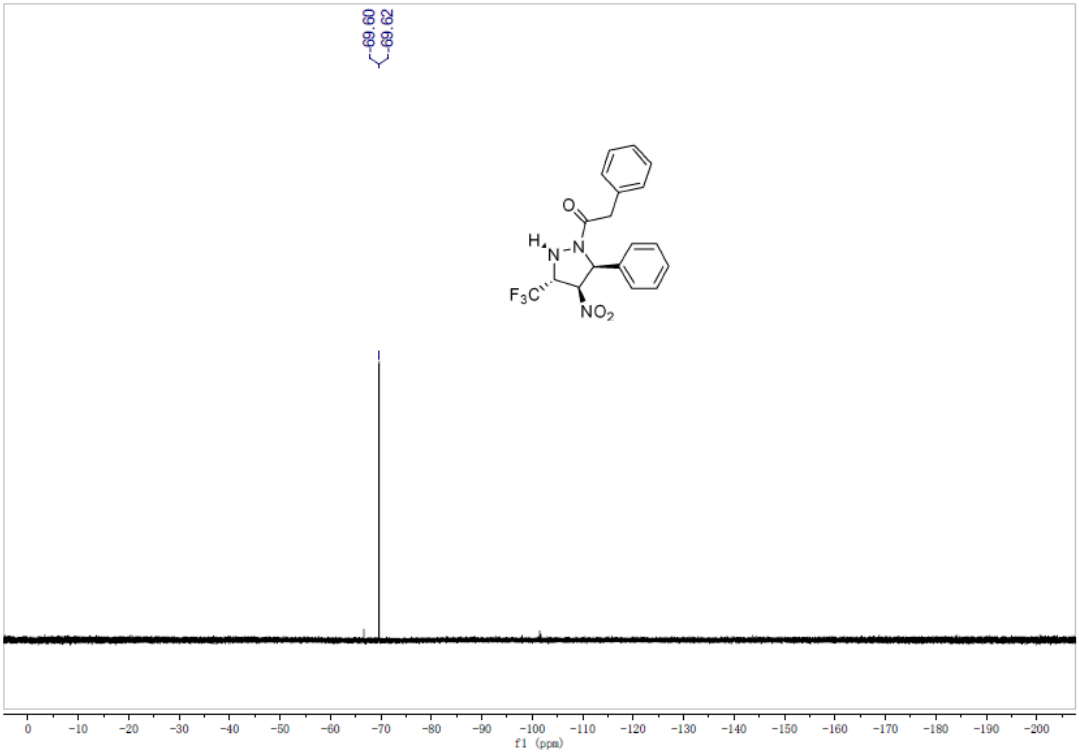
^{1}H NMR copies of compound **3oa**:



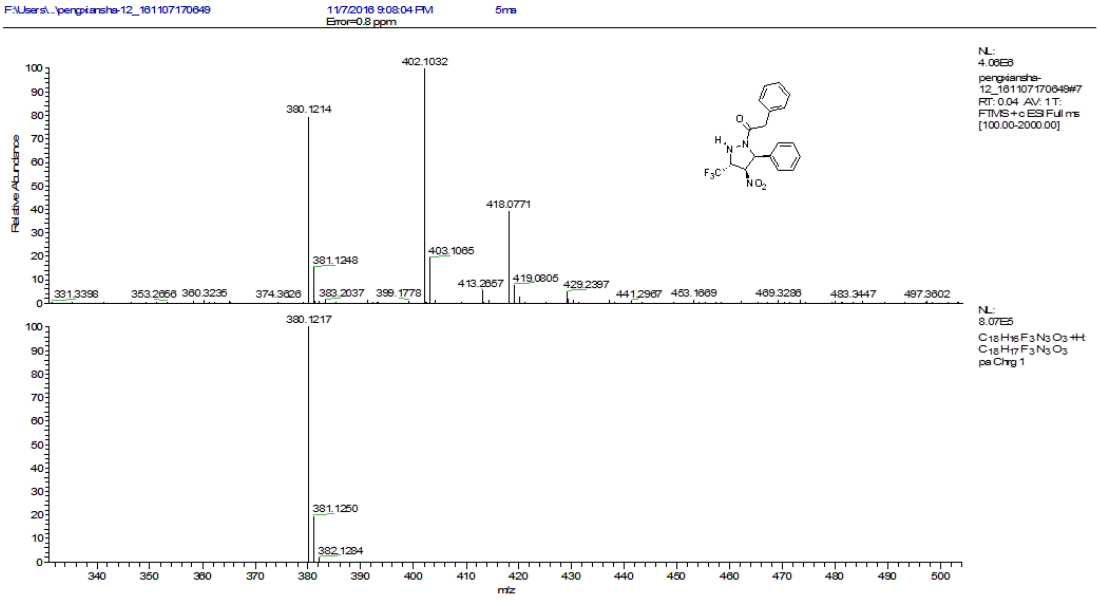
^{13}C NMR copies of compound **3oa**:



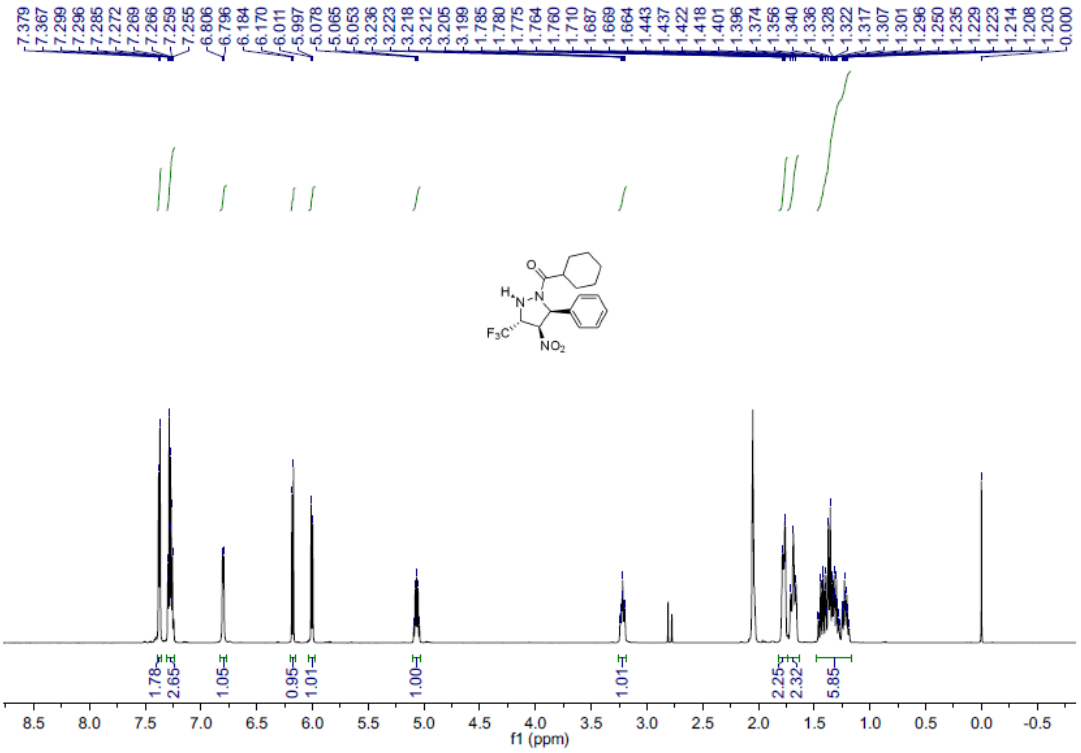
^{19}F NMR copies of compound **3oa**:



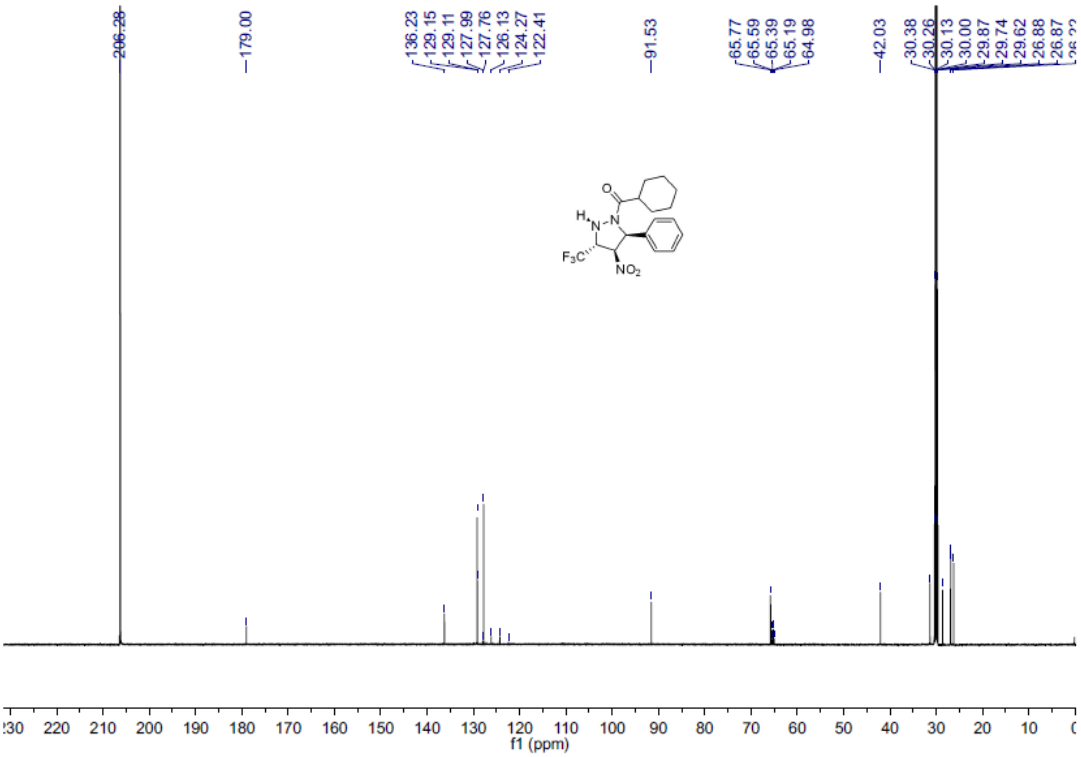
HRMS (ESI) of compound **3oa**:



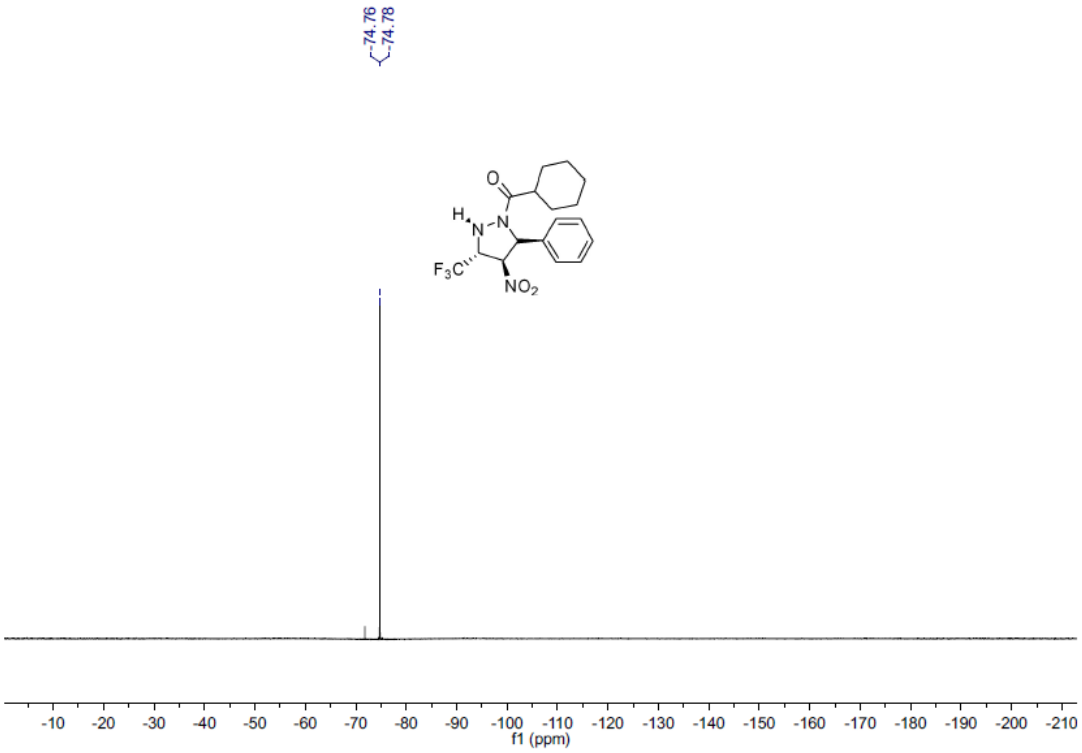
^{1}H NMR copies of compound **3pa**:



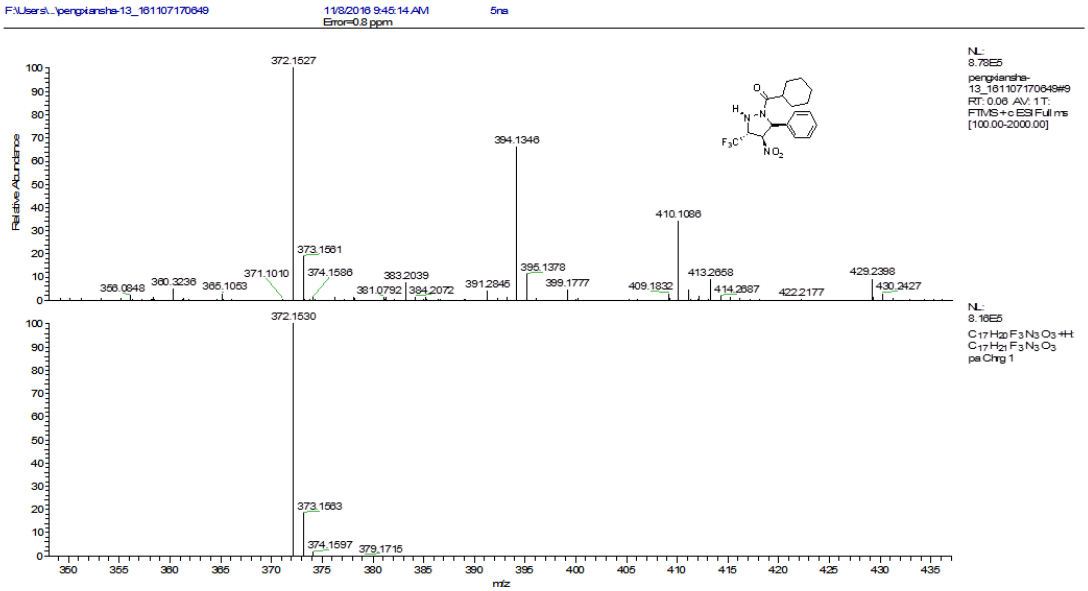
^{13}C NMR copies of compound **3pa**:



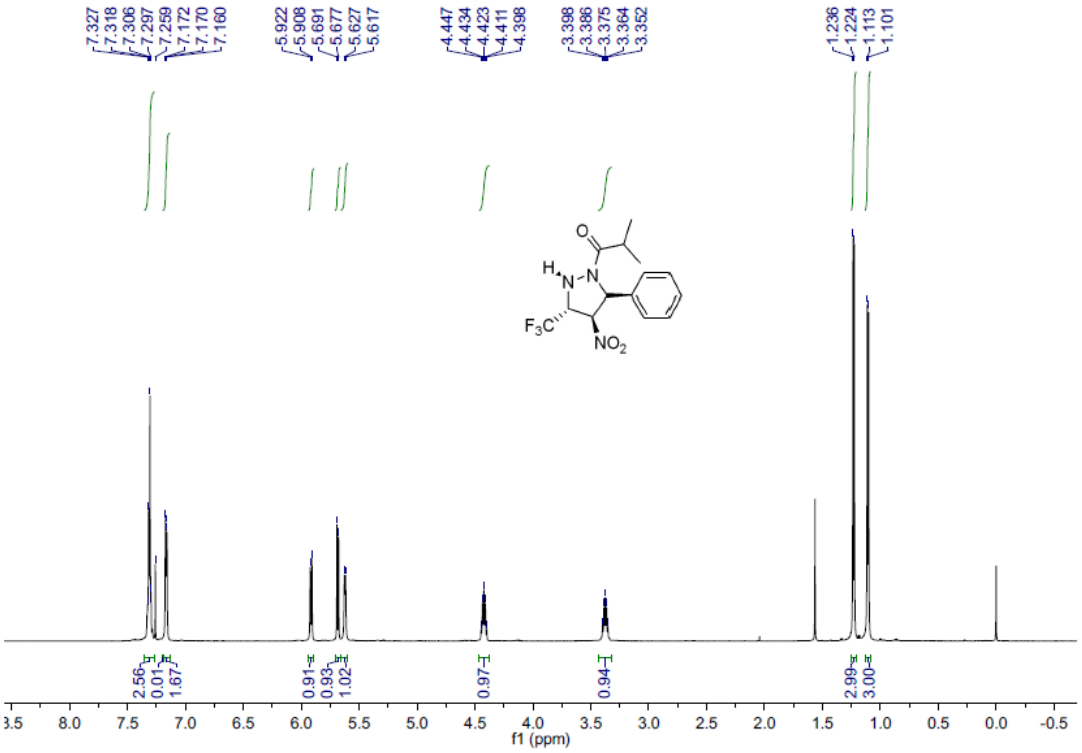
^{19}F NMR copies of compound **3pa**:



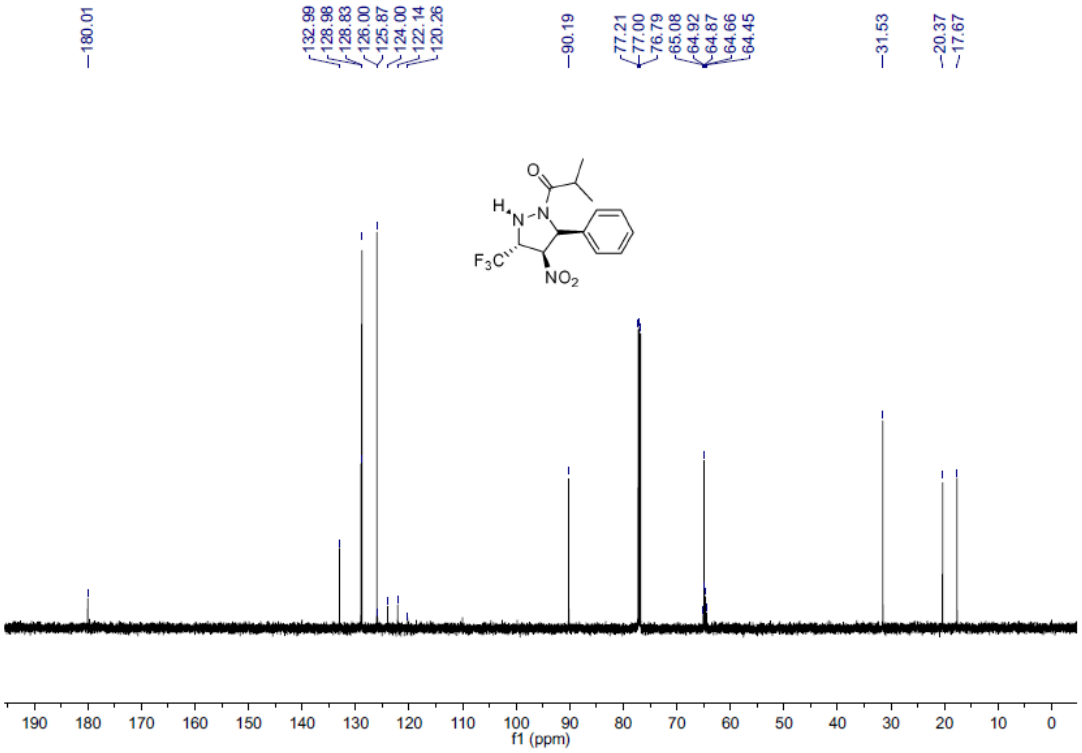
HRMS (ESI) of compound **3pa**:



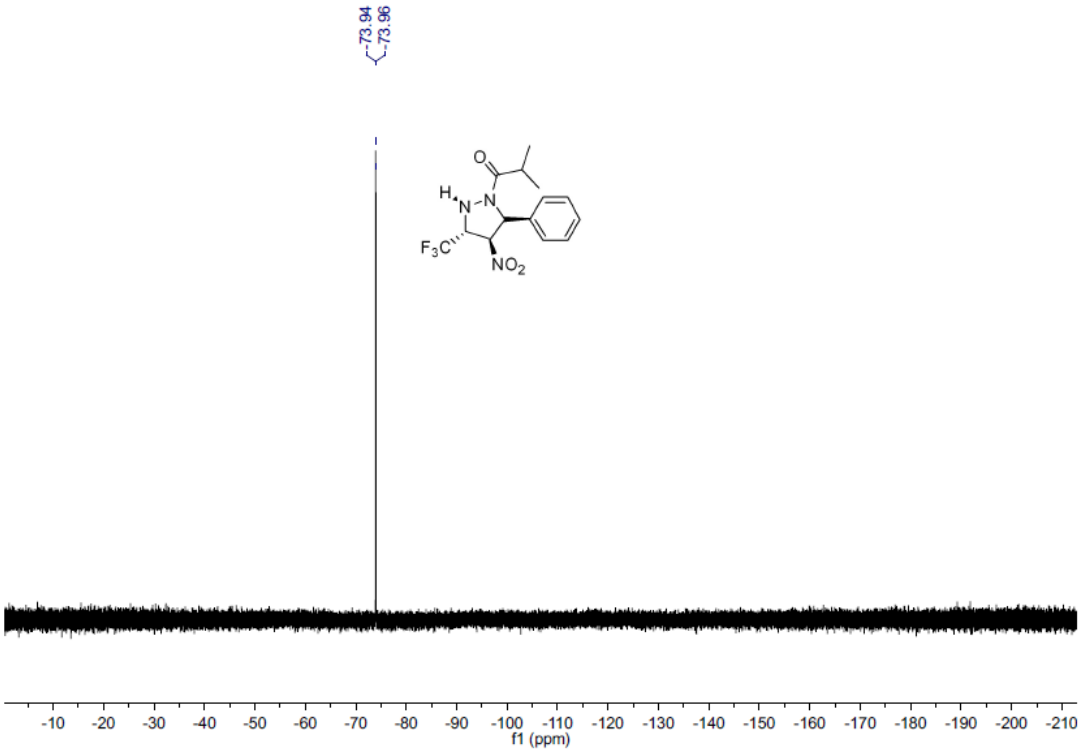
^{1}H NMR copies of compound **3qa**:



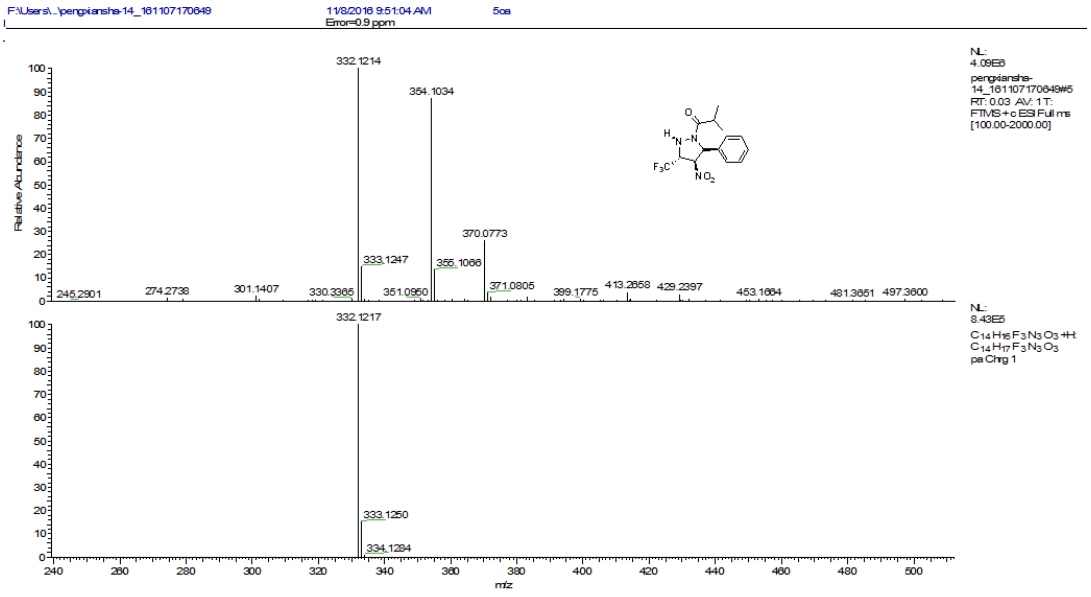
^{13}C NMR copies of compound **3qa**:



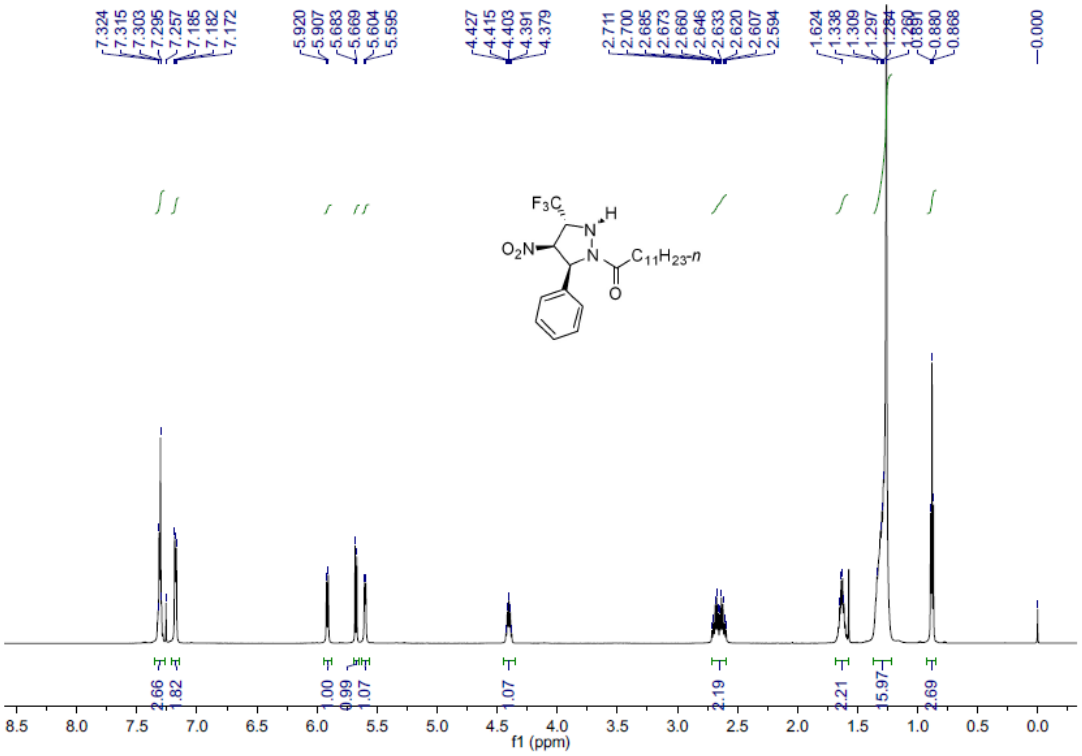
^{19}F NMR copies of compound **3qa**:



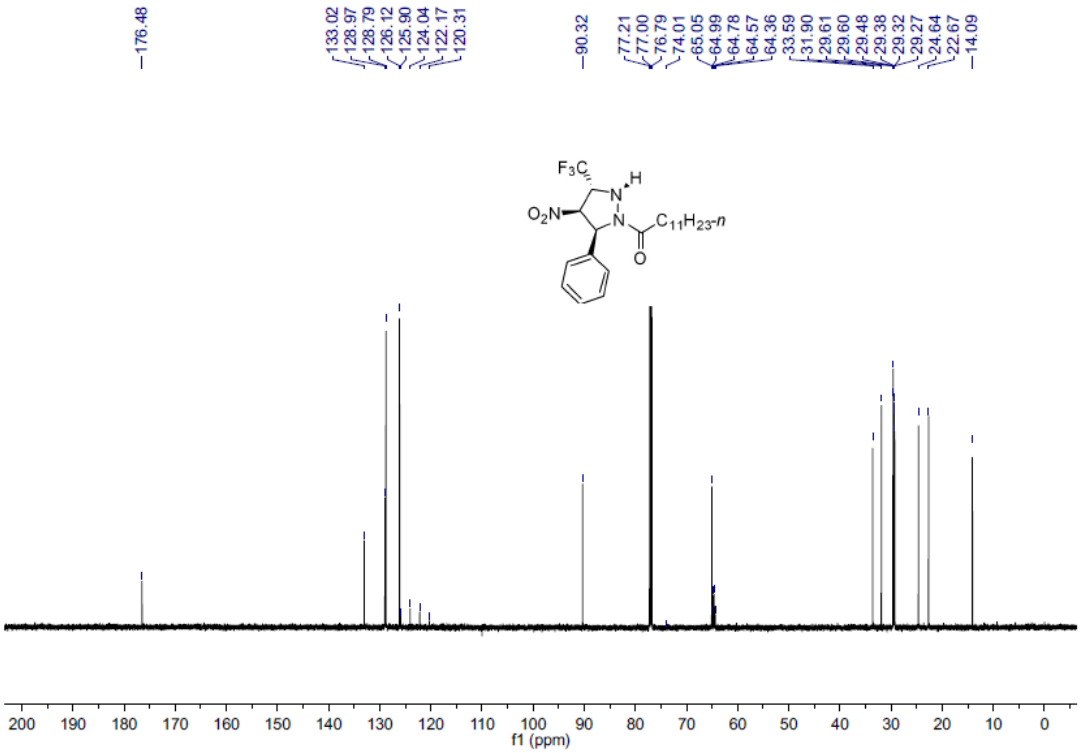
HRMS (ESI) of compound **3qa**:

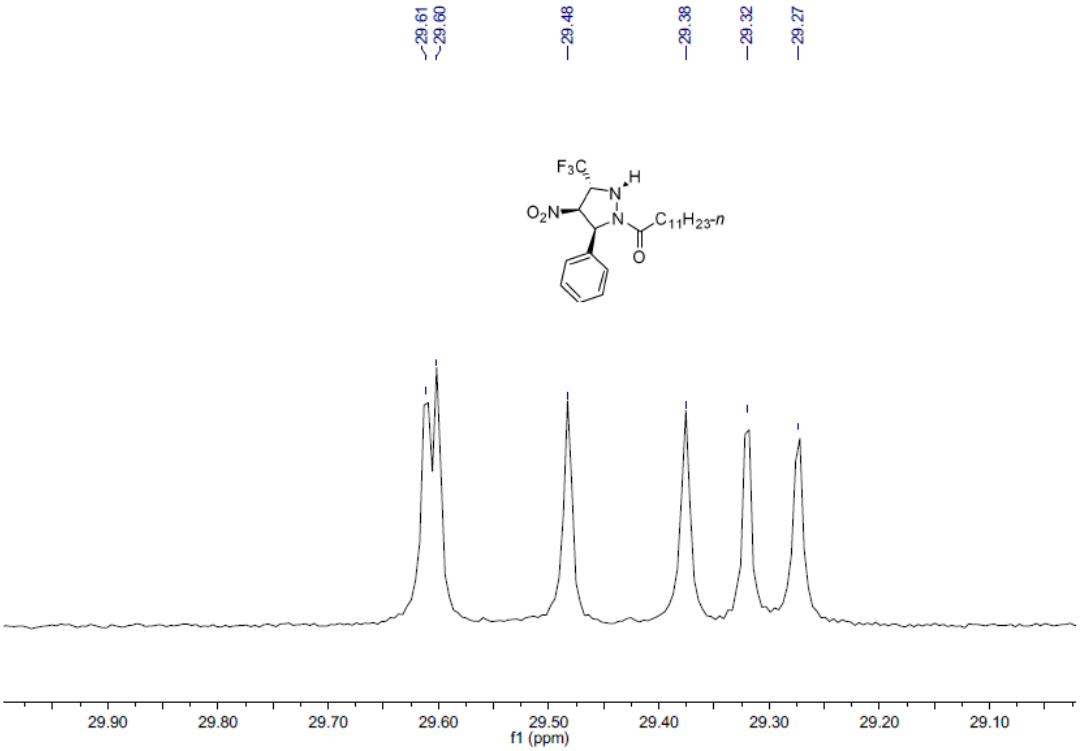


^{1}H NMR copies of compound **3ra**:

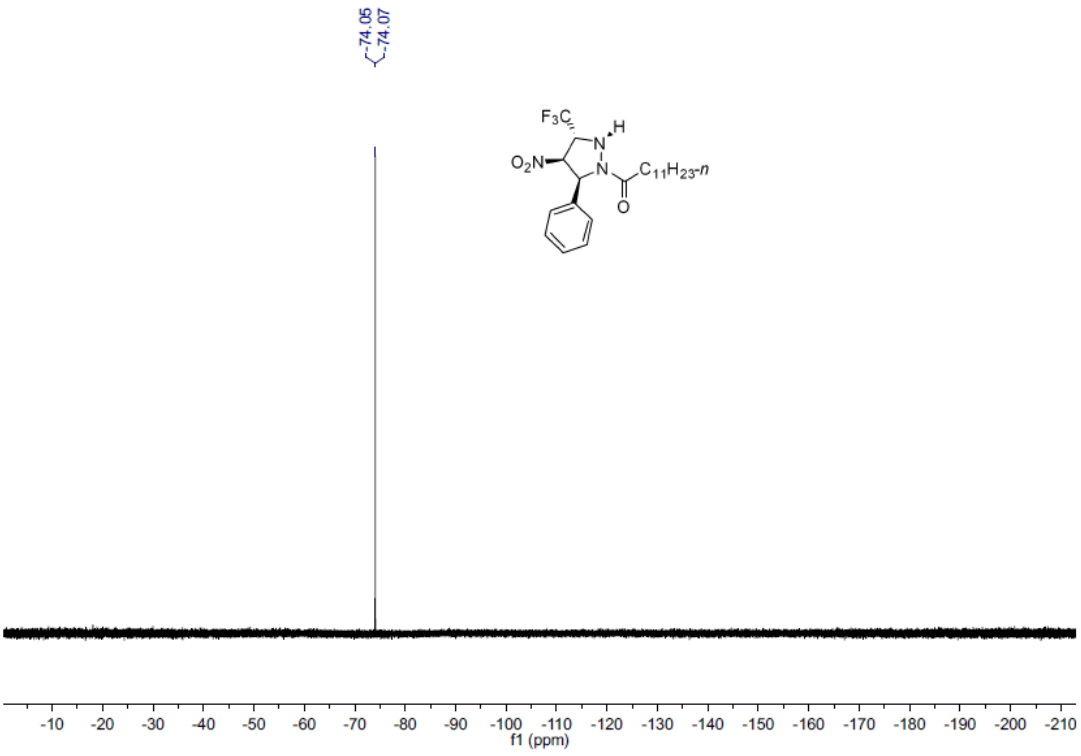


^{13}C NMR copies of compound **3ra**:

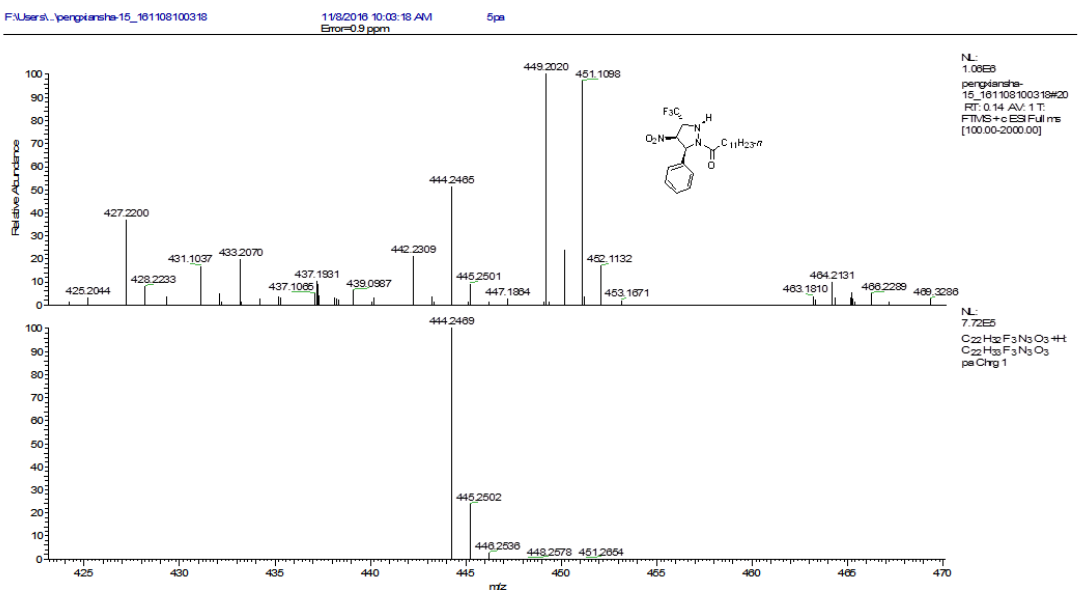




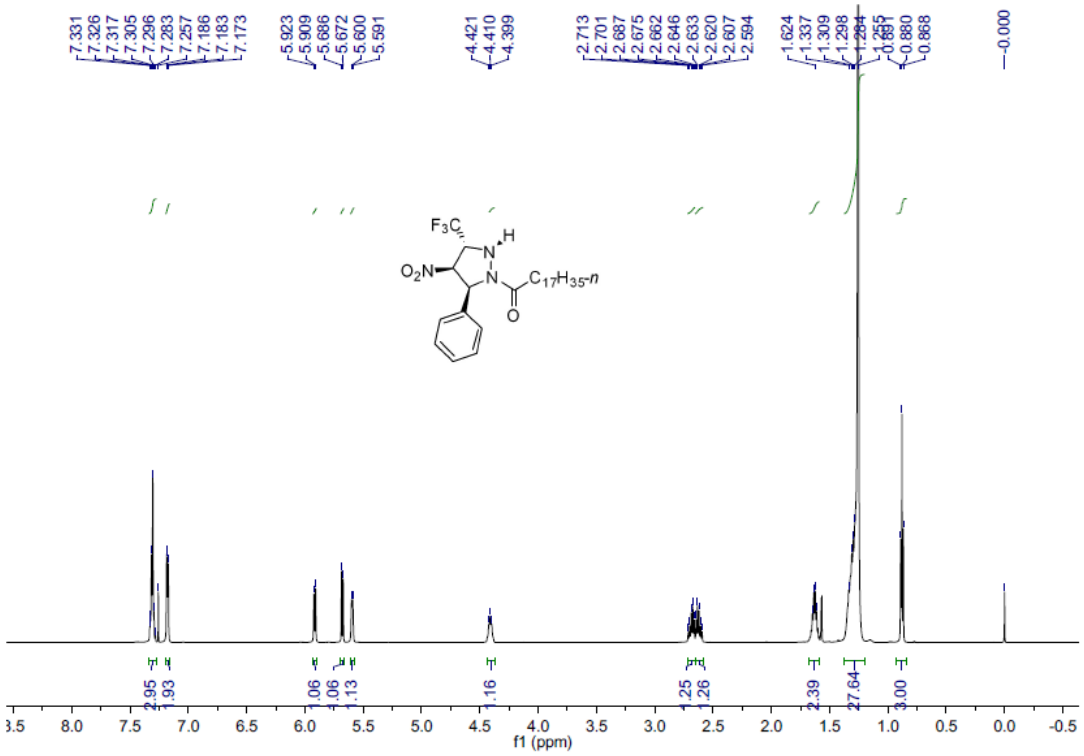
^{19}F NMR copies of compound **3ra**:



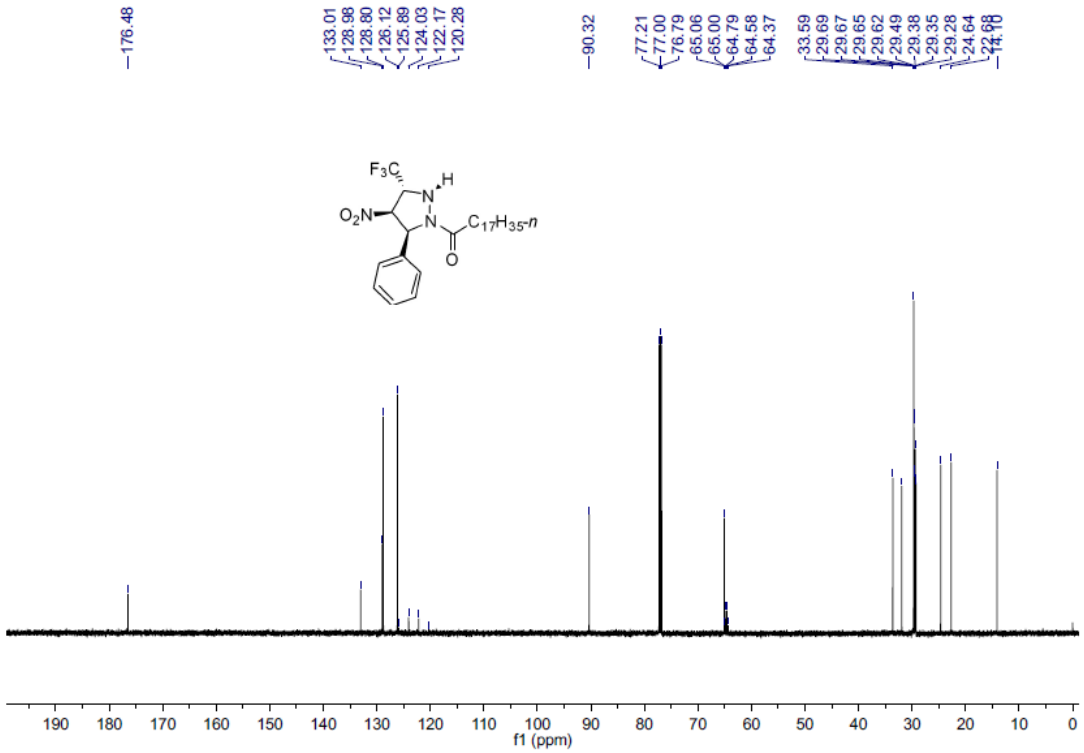
HRMS (ESI) of compound **3ra**:

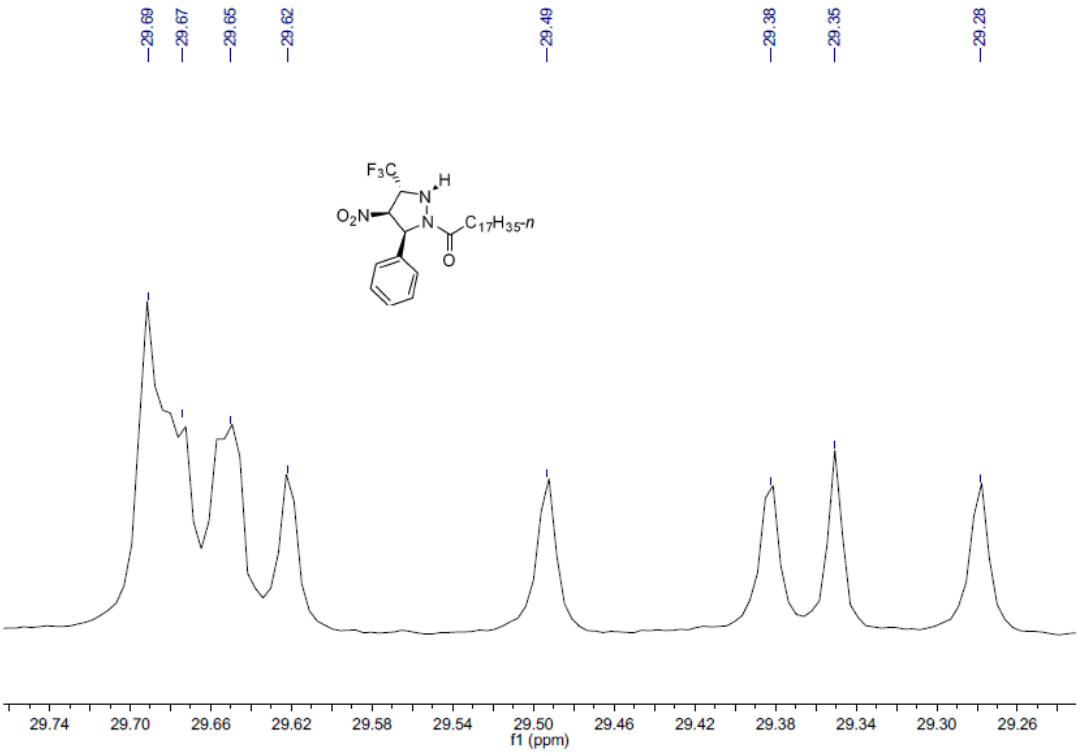

F:\Users\..\pengxiansha-15_161108100318
11/8/2016 10:03:18 AM
5pa
Error=0.9 ppm
NL:
1.08E8
pengxiansha-15_161108100318#20
RT: 0.14 AV: 1 T:
FTMS + c ESI Full ms
[100.00-2000.00]
449.2020
451.1098
444.2485
427.2200
431.1037
433.2070
442.2309
437.1931
437.1065
439.0987
445.2501
447.1984
452.1132
453.1671
425.2044
428.2233
463.1810
464.2131
466.2289
468.3286
Relative Abundance
NL:
7.72E5
C22 H32 F3 N3 O3 +H
C22 H33 F3 N3 O3
pa Chrg 1
444.2489
445.2502
446.2536
448.2578
451.2654
m/z

^{1}H NMR copies of compound **3sa**:

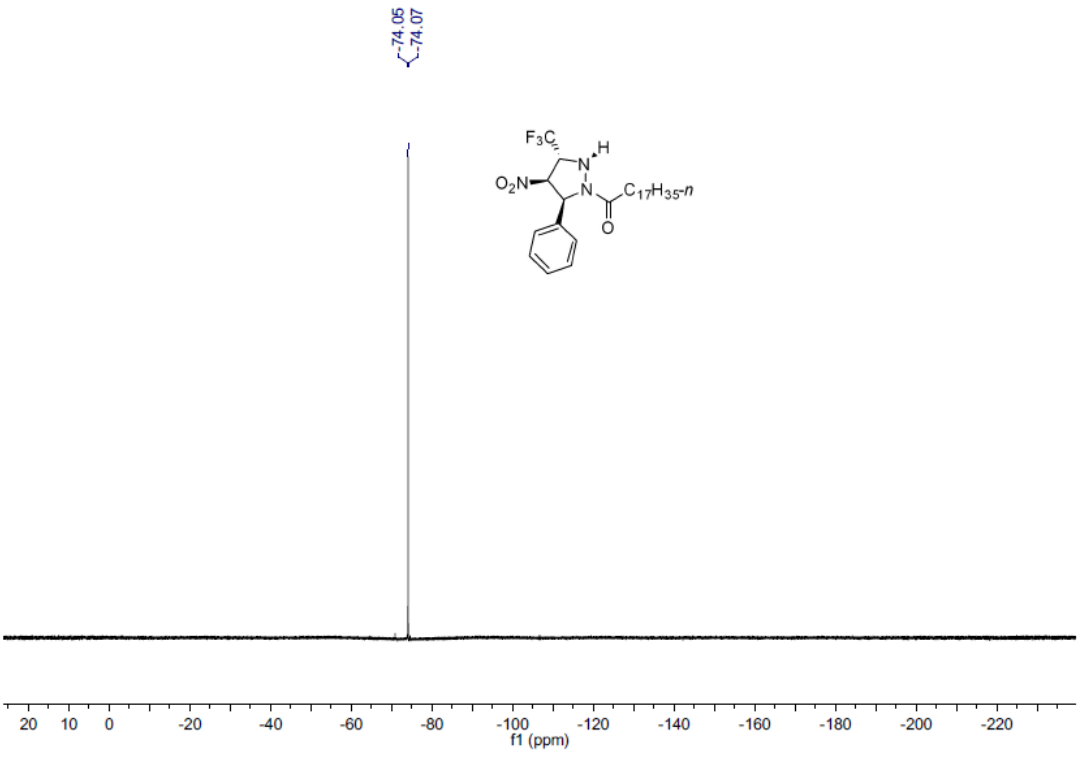


^{13}C NMR copies of compound **3sa**:

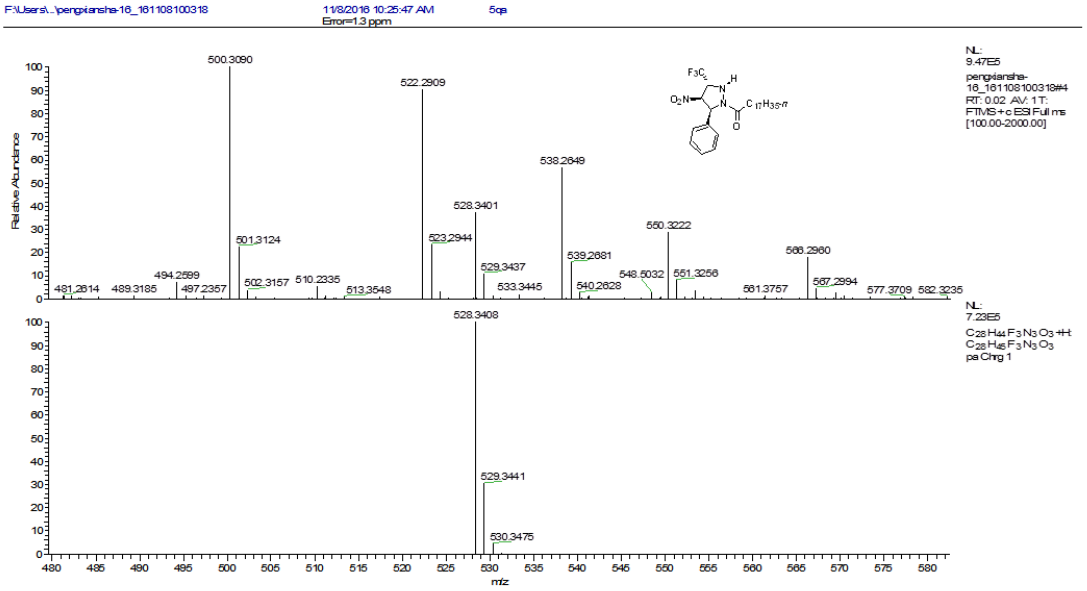




^{19}F NMR copies of compound **3sa**:

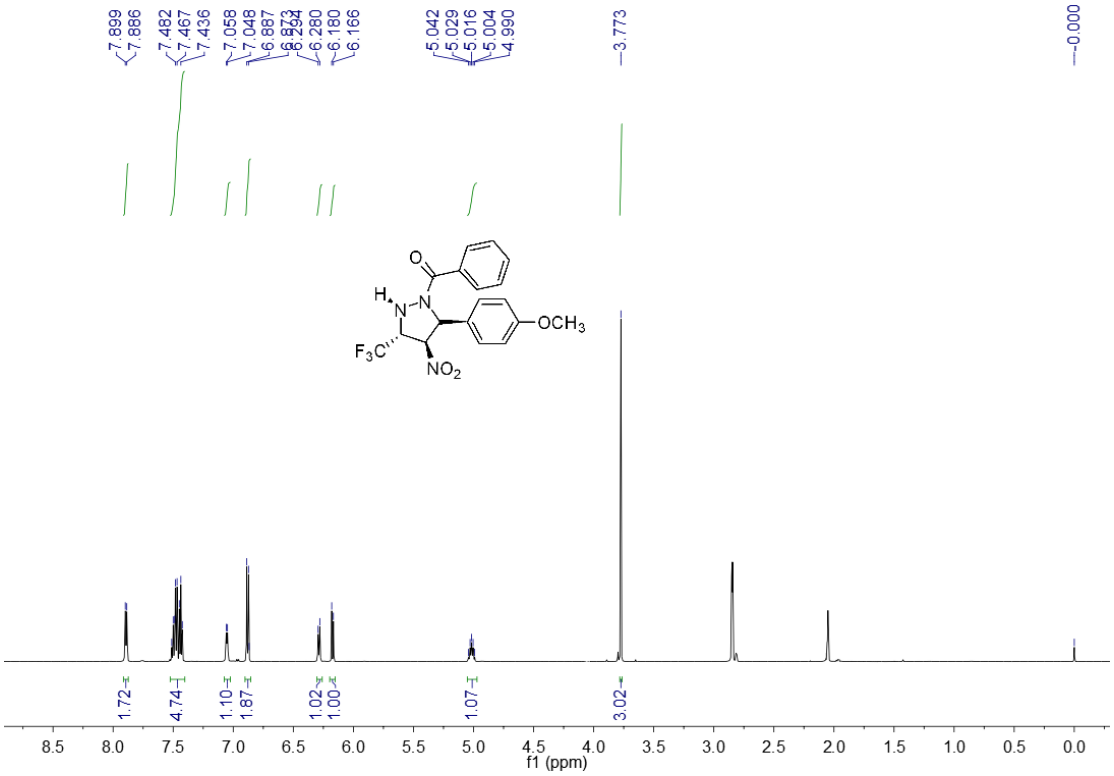


HRMS (ESI) of compound **3sa**:

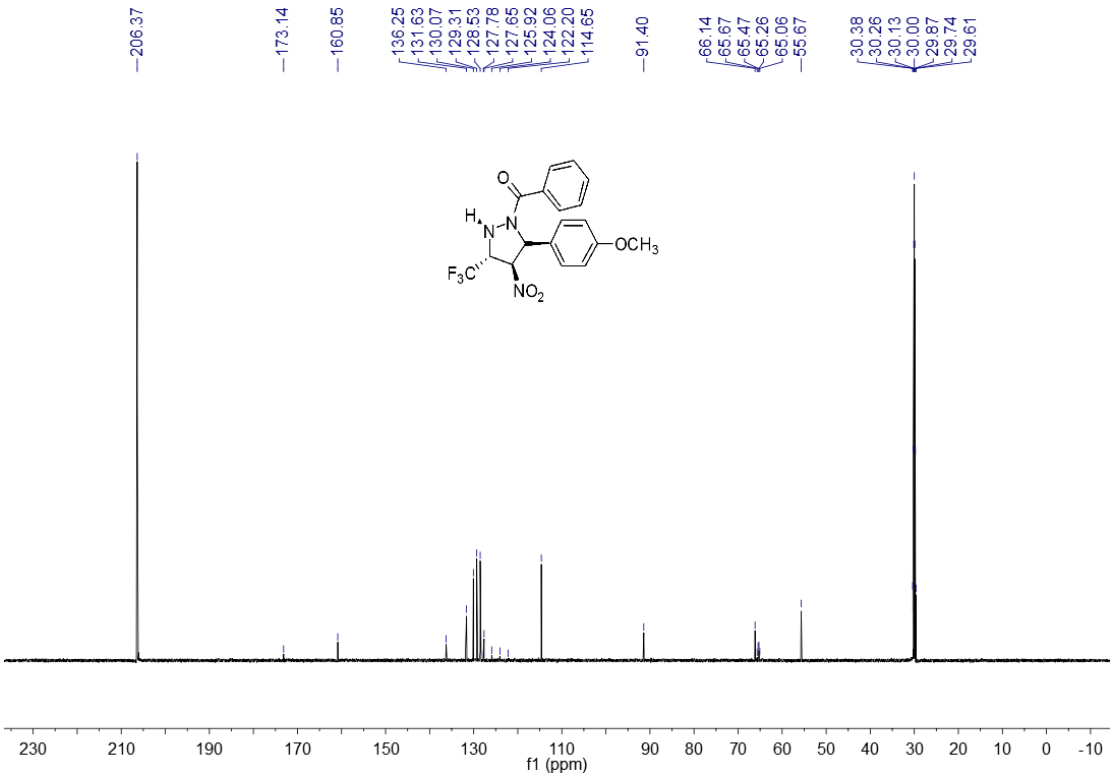


7 NMR, HRMS copies of compounds 3ab-3ao

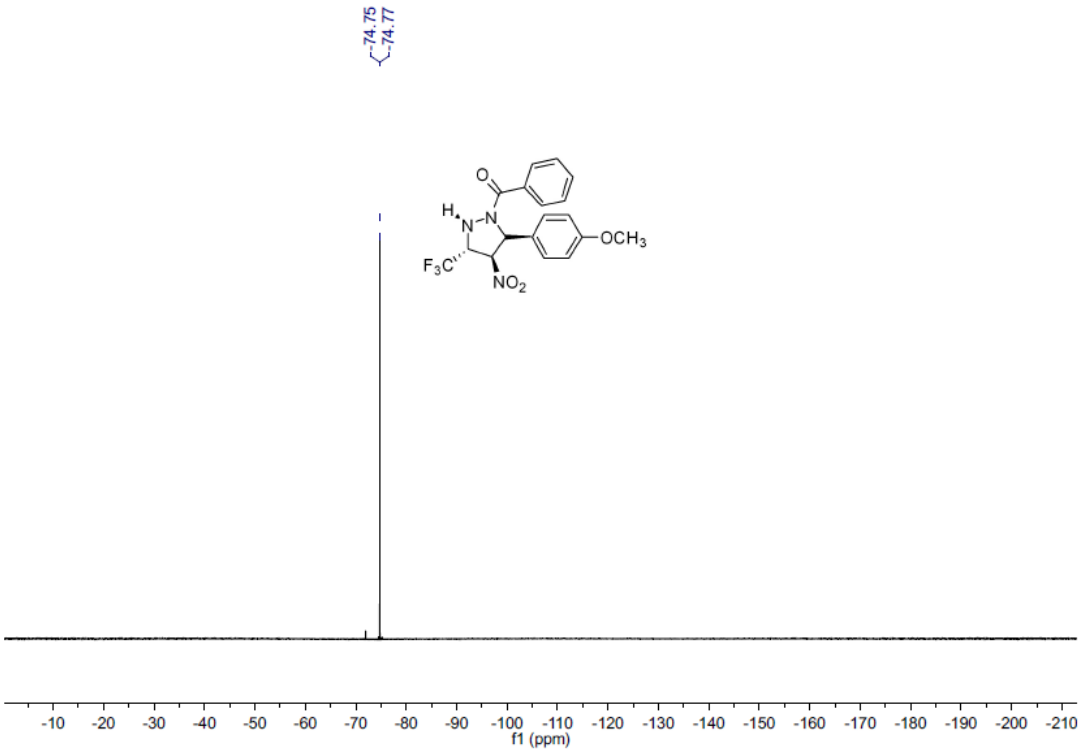
^{1}H NMR copies of compound **3ab**:



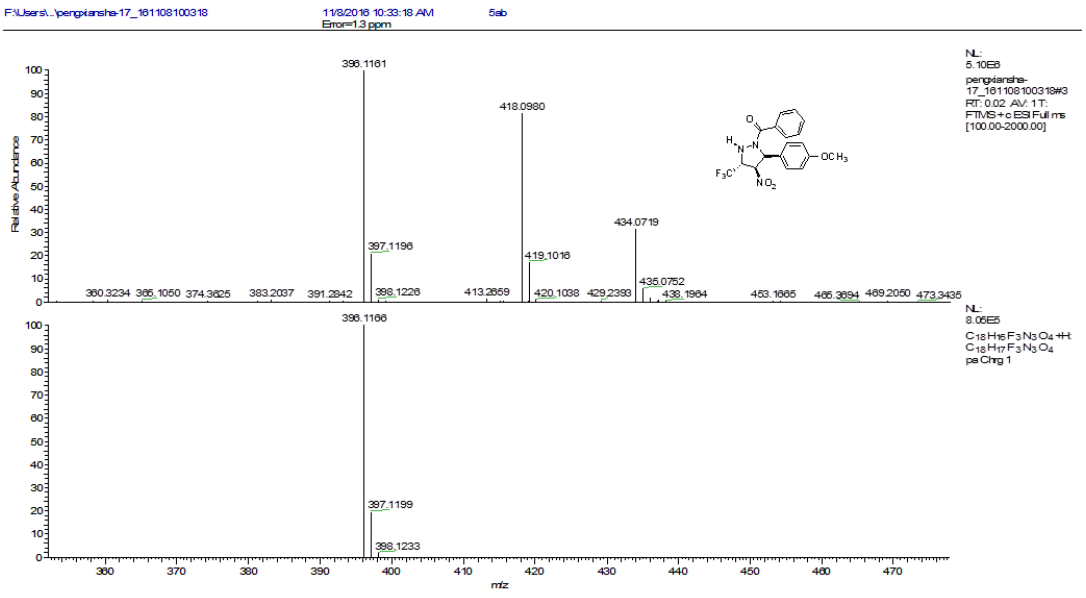
^{13}C NMR copies of compound **3ab**:



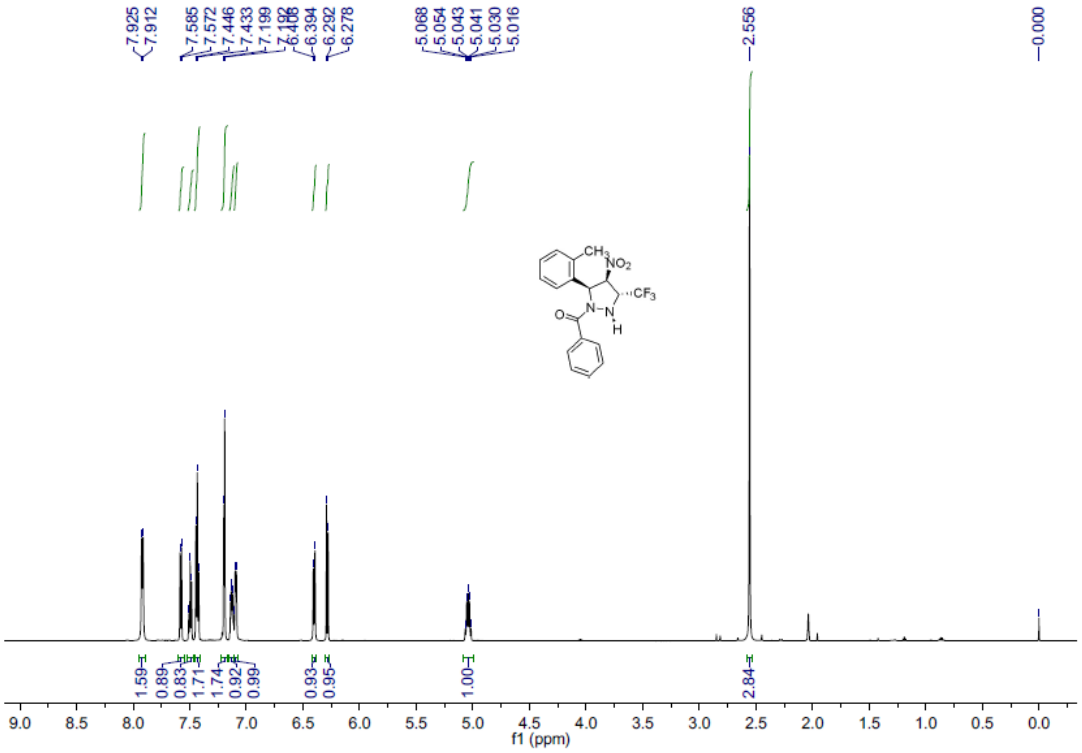
^{19}F NMR copies of compound **3ab**:



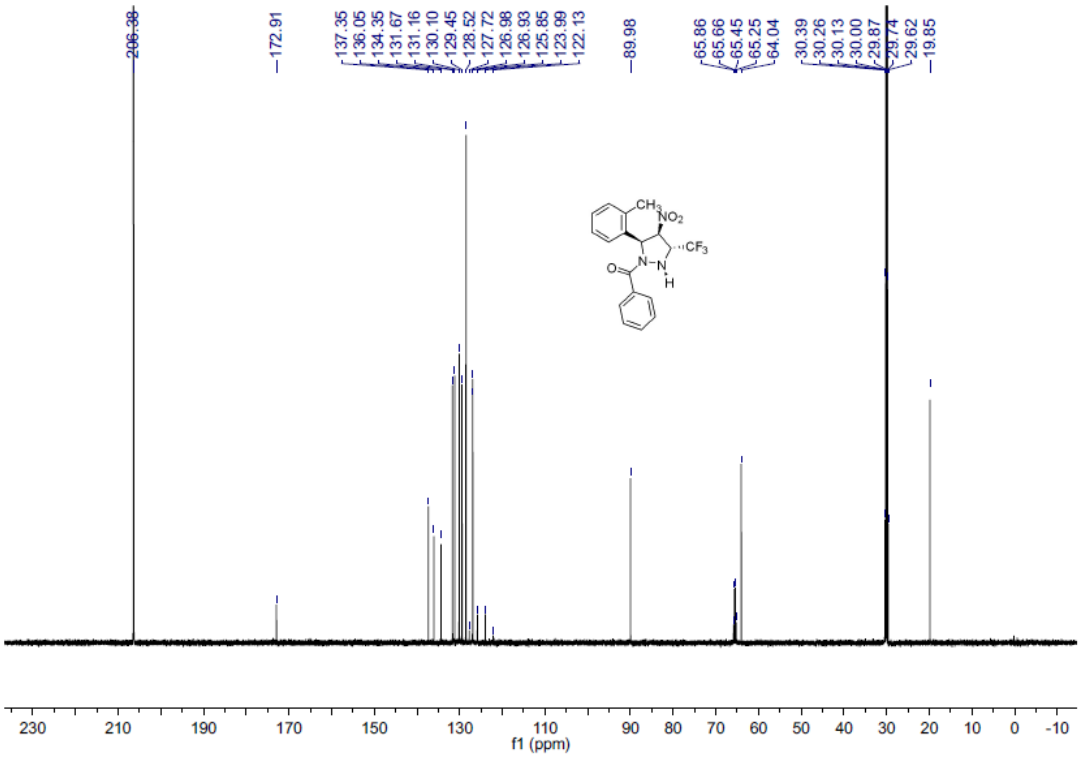
HRMS (ESI) of compound **3ab**:



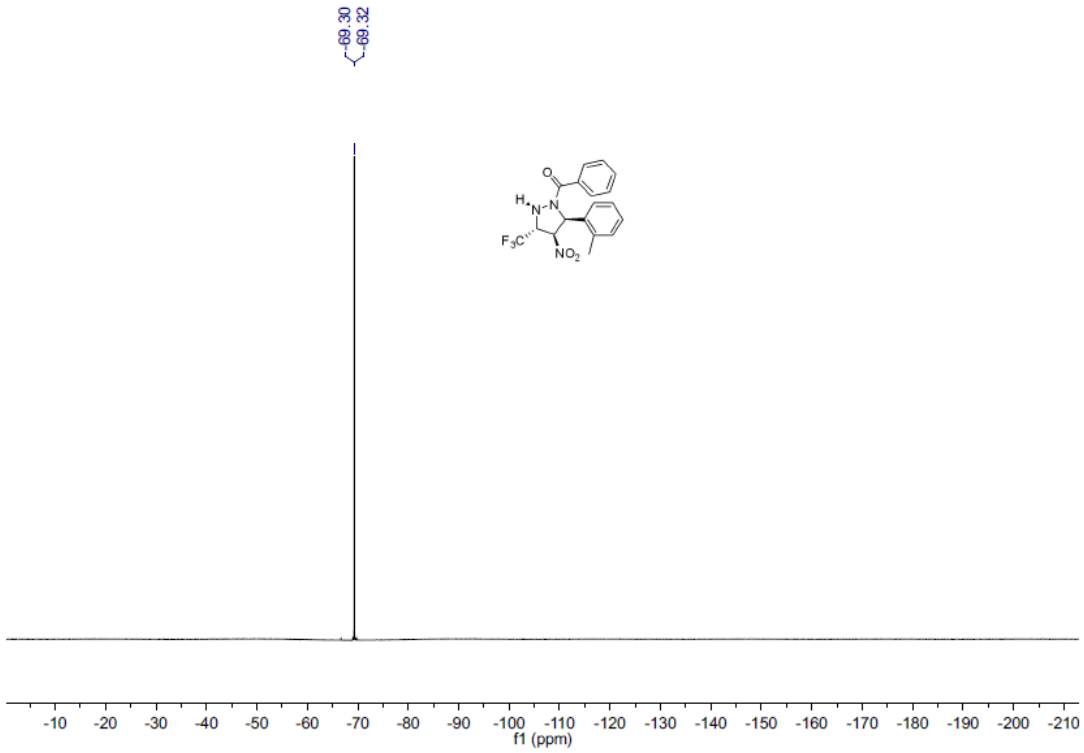
^{1}H NMR copies of compound **3ac**:



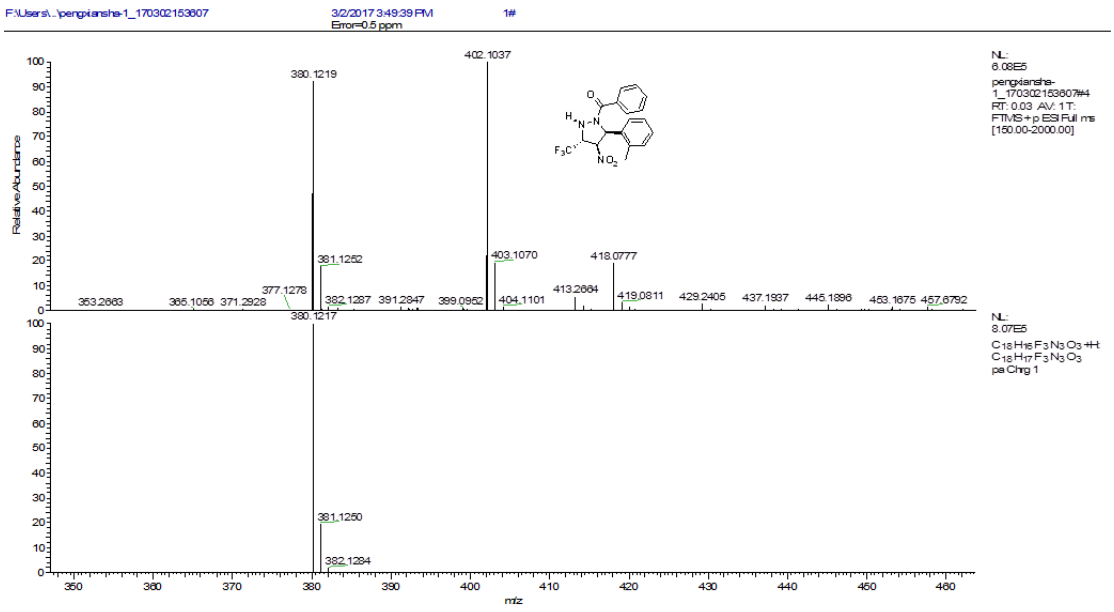
^{13}C NMR copies of compound **3ac**:



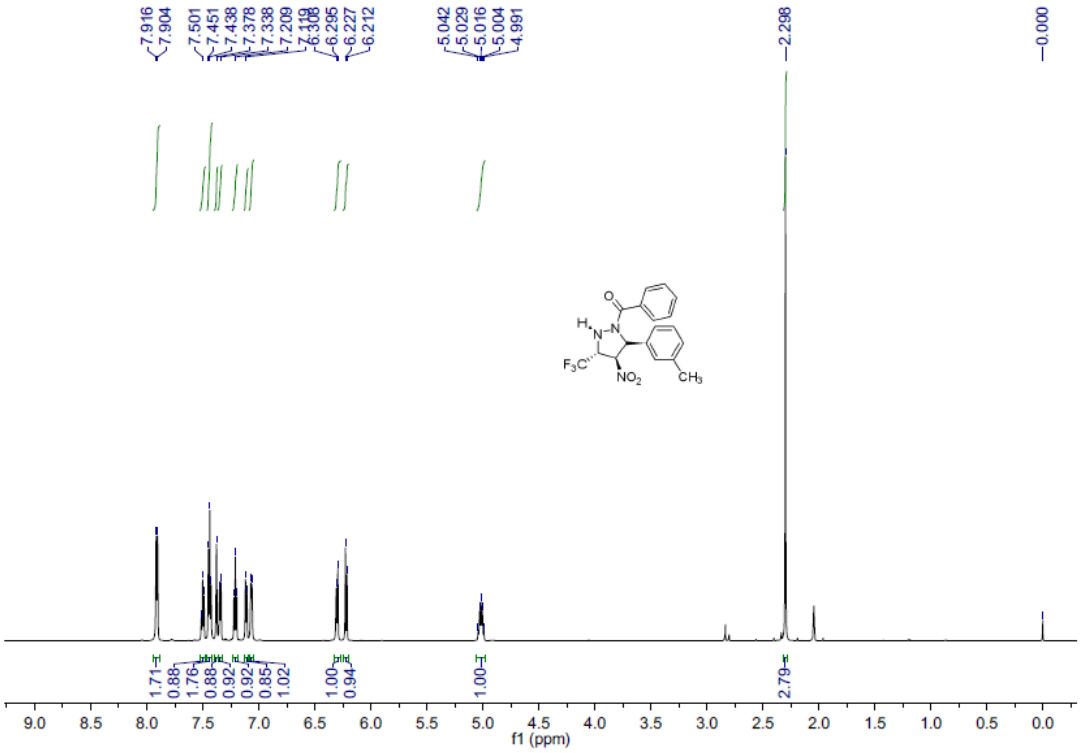
^{19}F NMR copies of compound **3ac**:



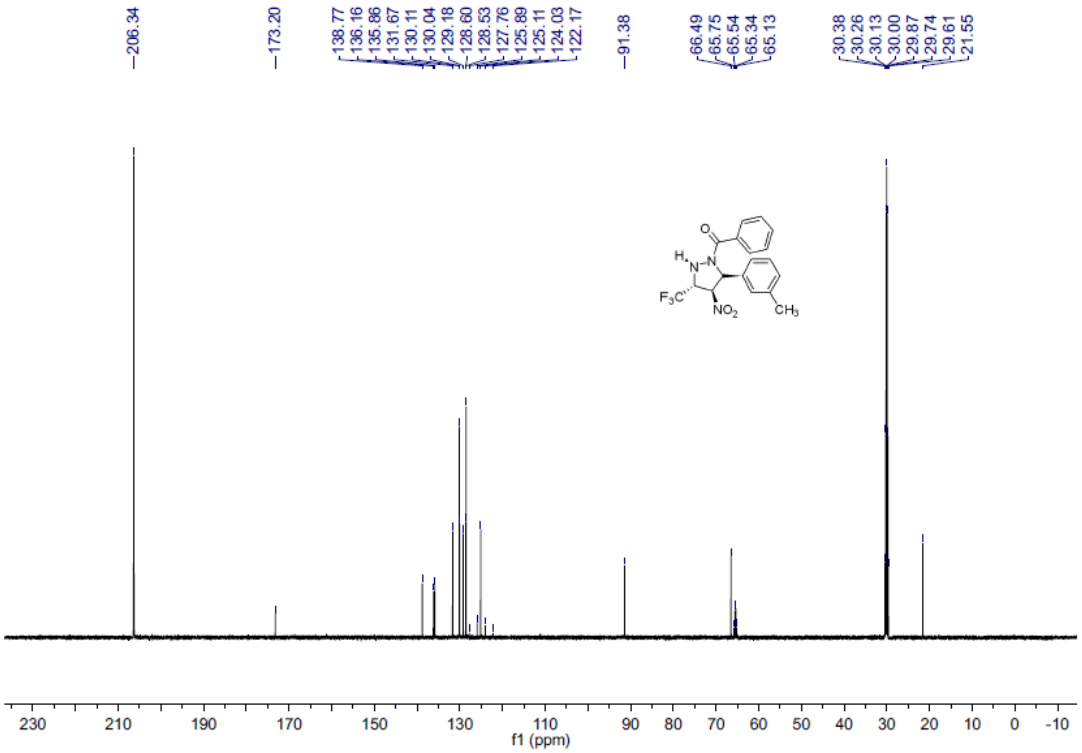
HRMS (ESI) of compound **3ac**:



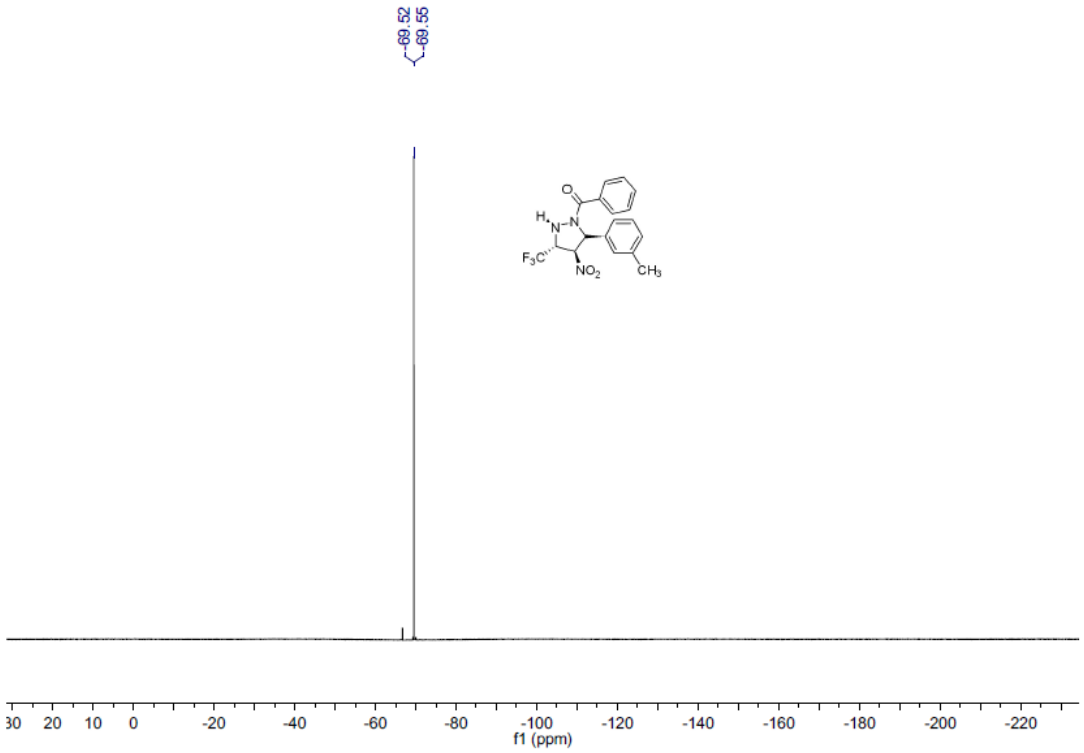
^{1}H NMR copies of compound **3ad**:



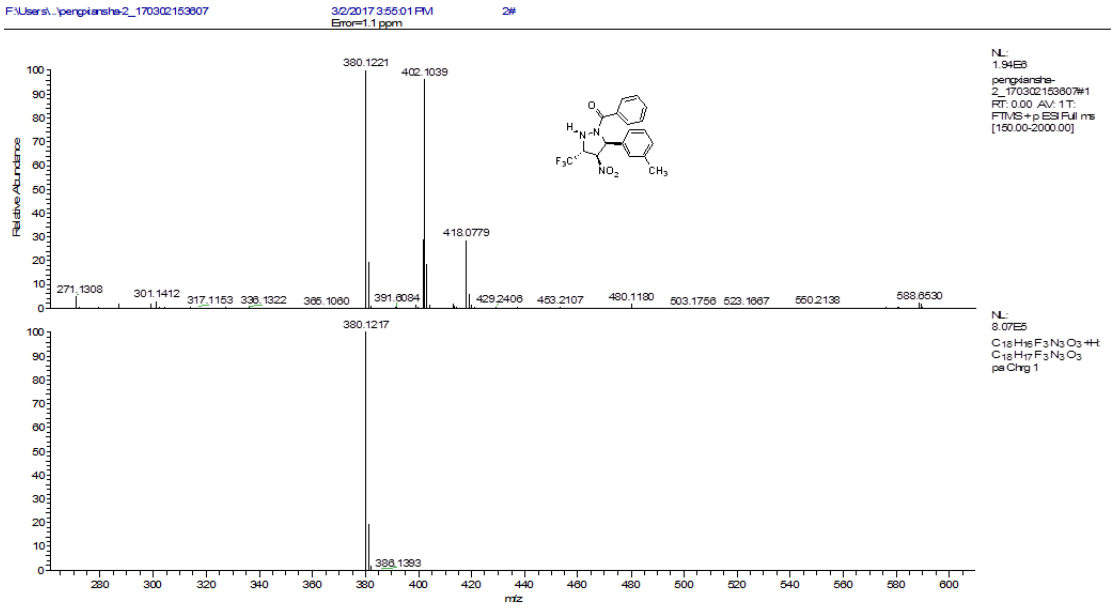
^{13}C NMR copies of compound **3ad**:



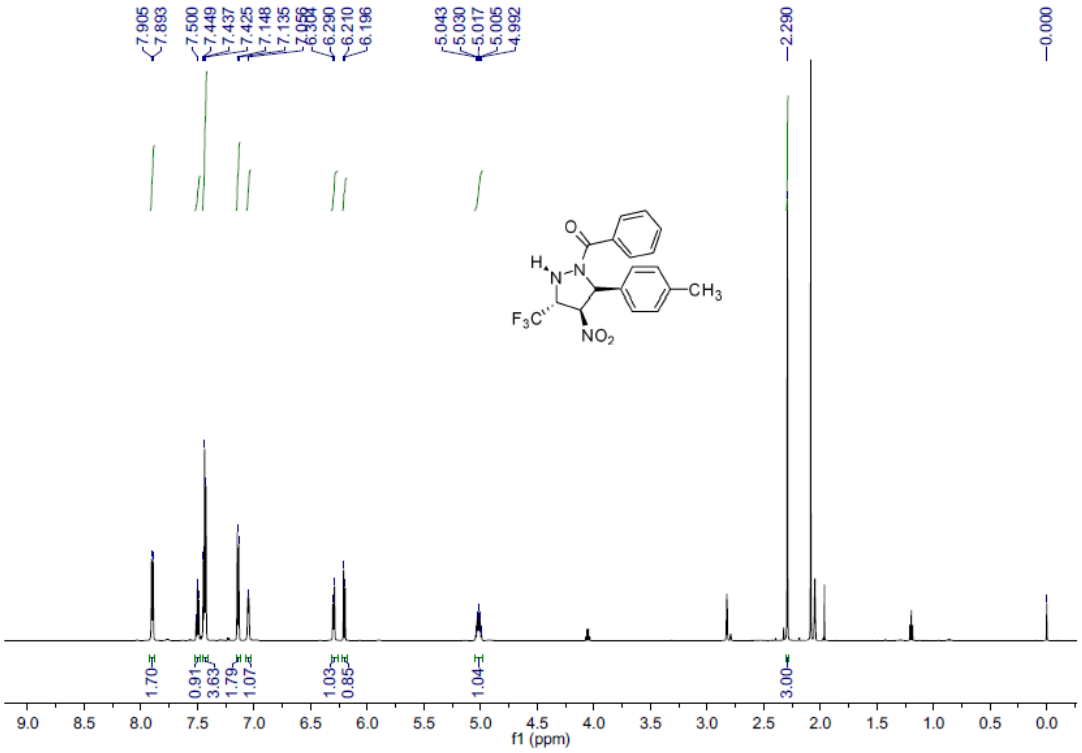
^{19}F NMR copies of compound **3ad**:



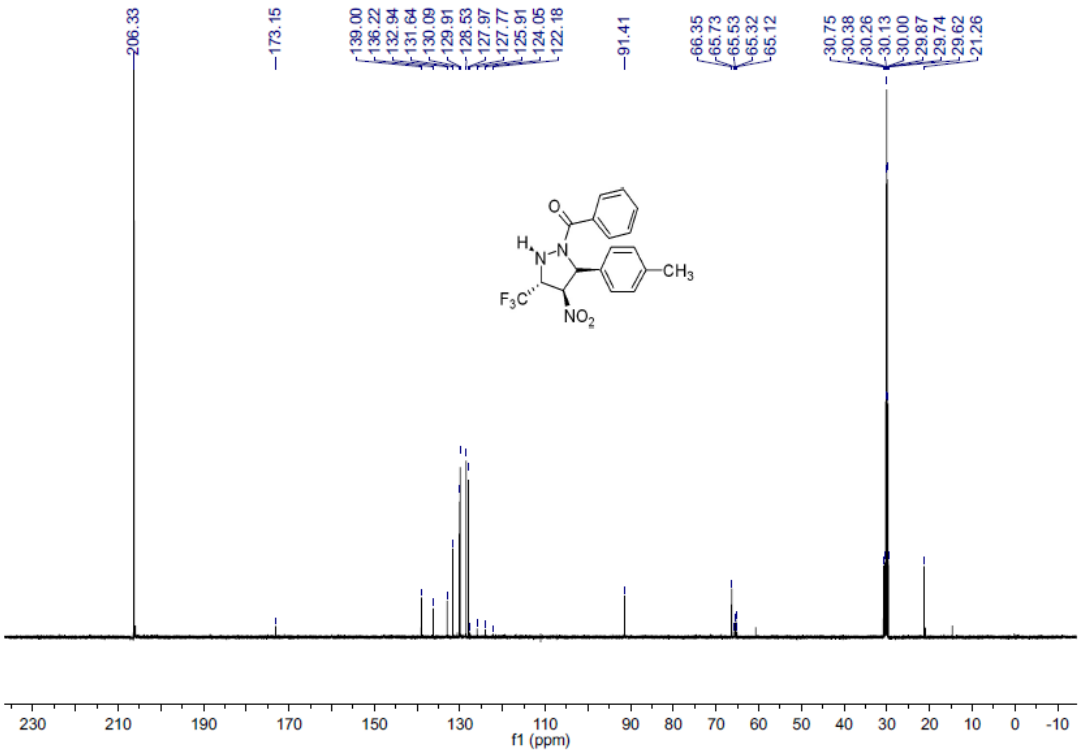
HRMS (ESI) of compound **3ad**:



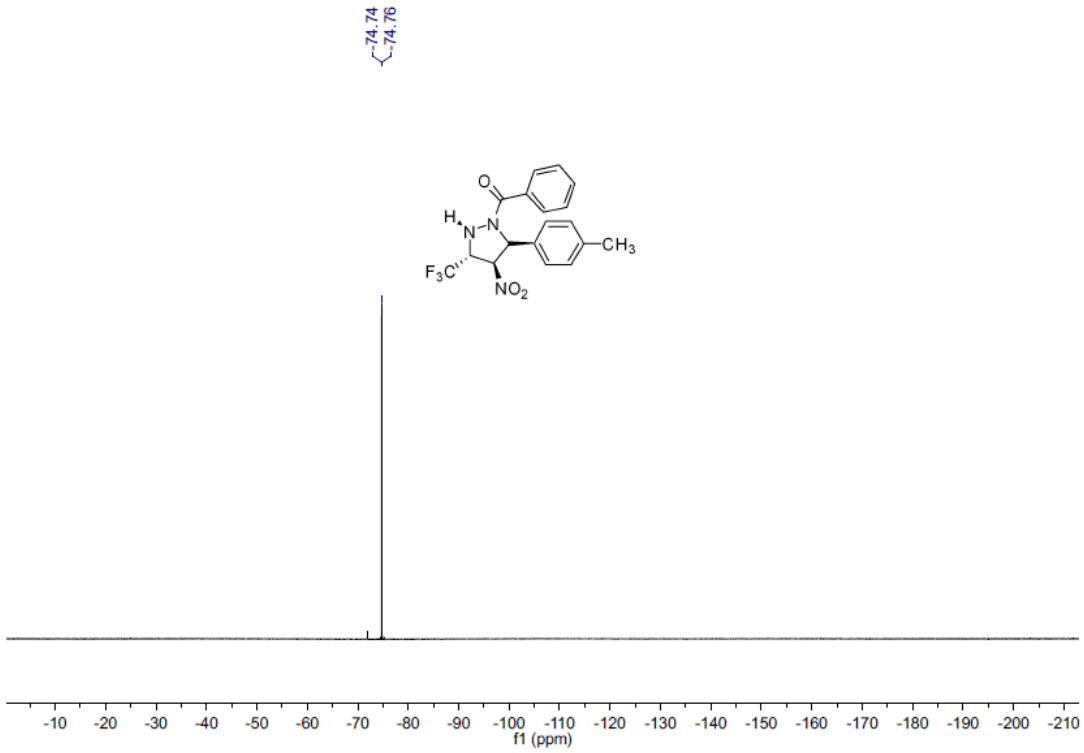
^{1}H NMR copies of compound **3ae**:



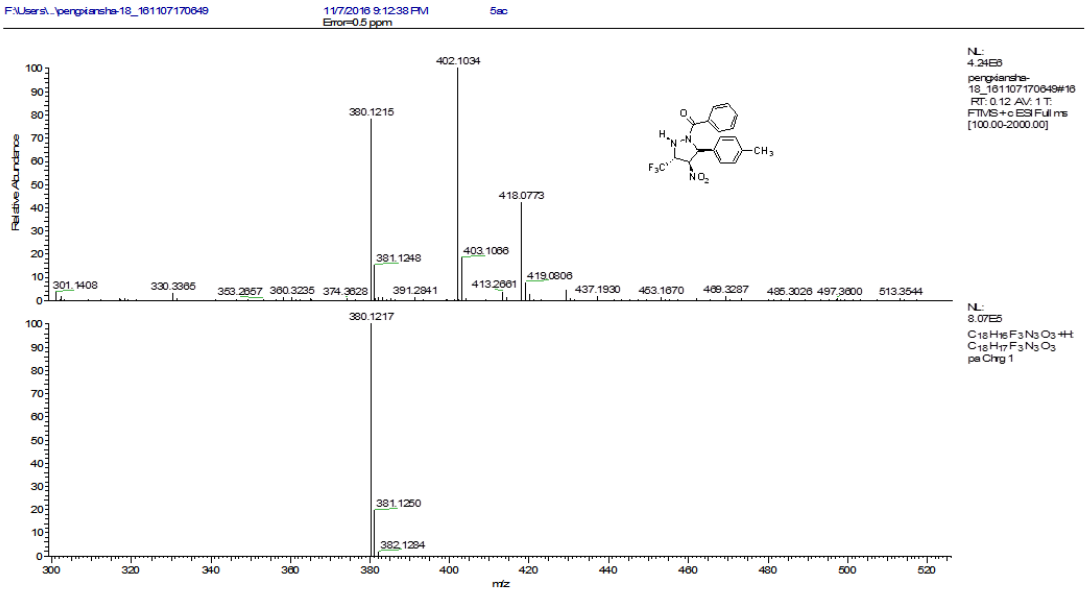
^{13}C NMR copies of compound **3ae**:



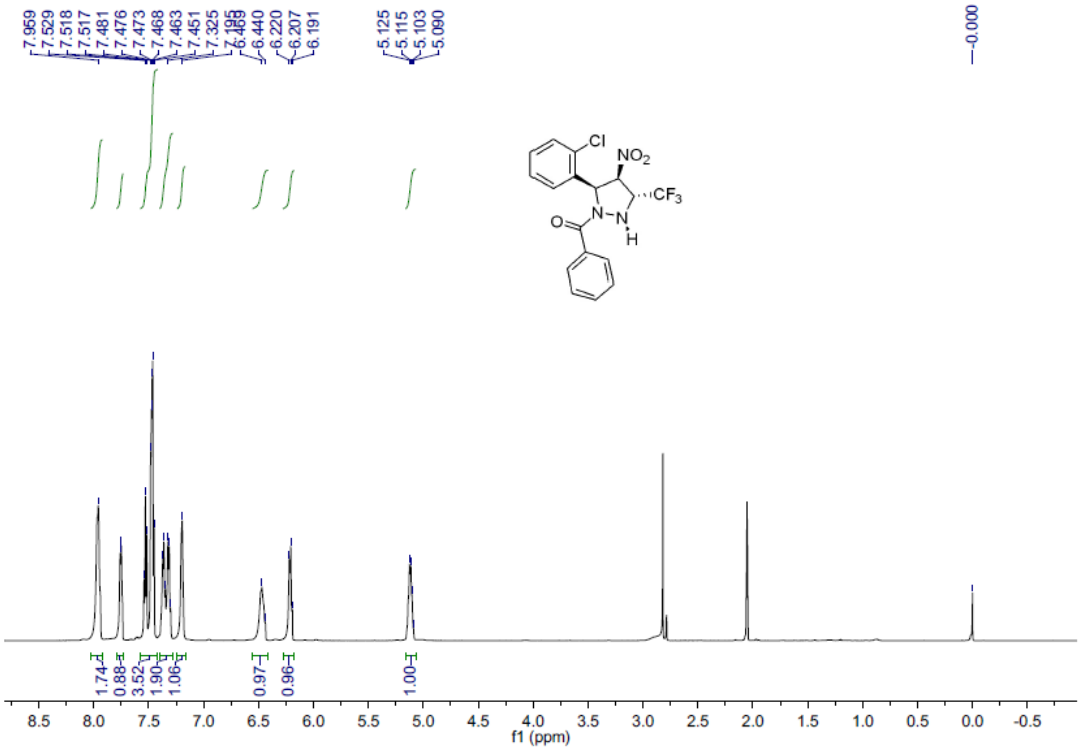
^{19}F NMR copies of compound **3ae**:



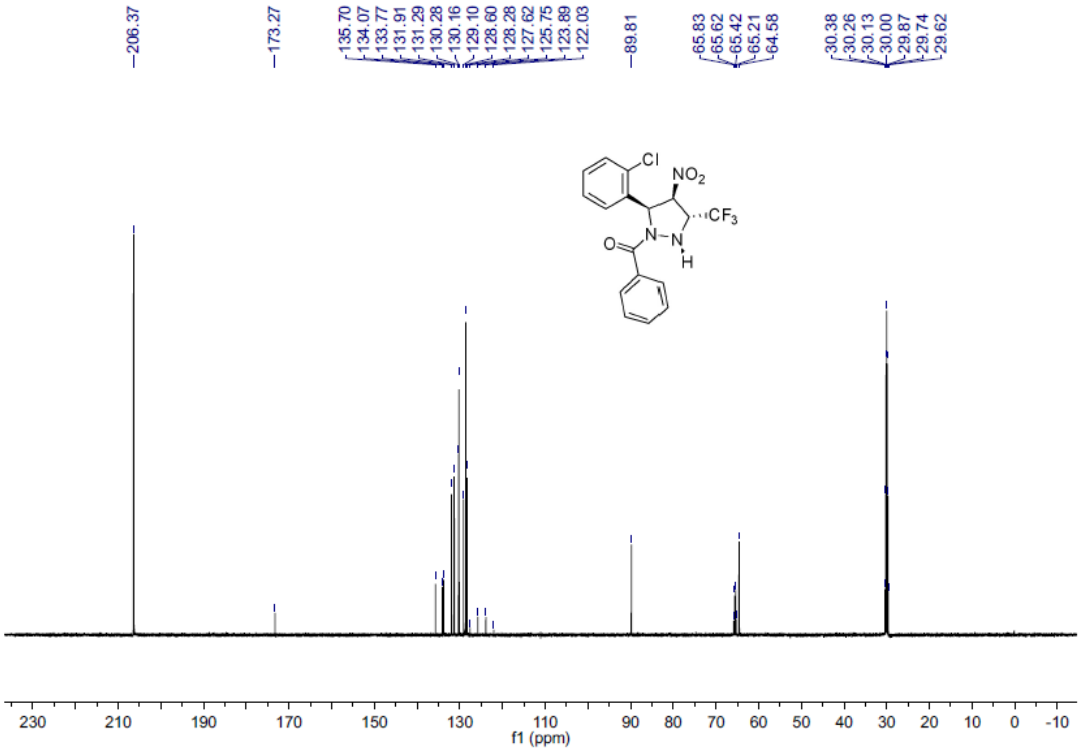
HRMS (ESI) of compound **3ae**:



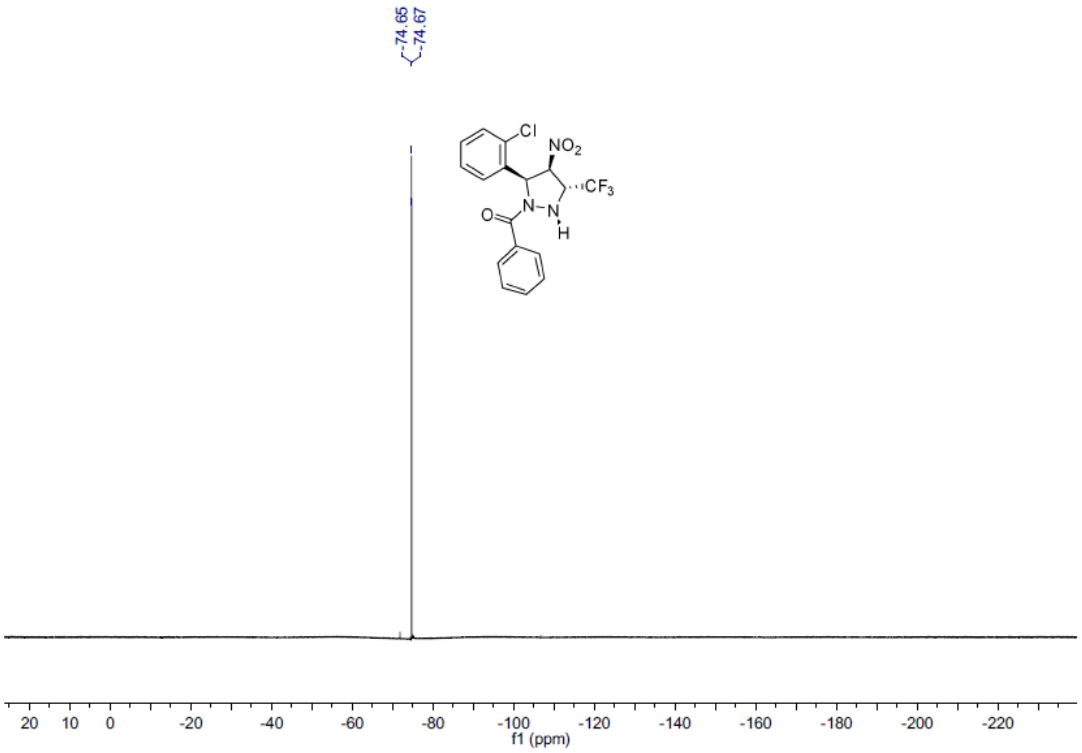
^{1}H NMR copies of compound **3af**:



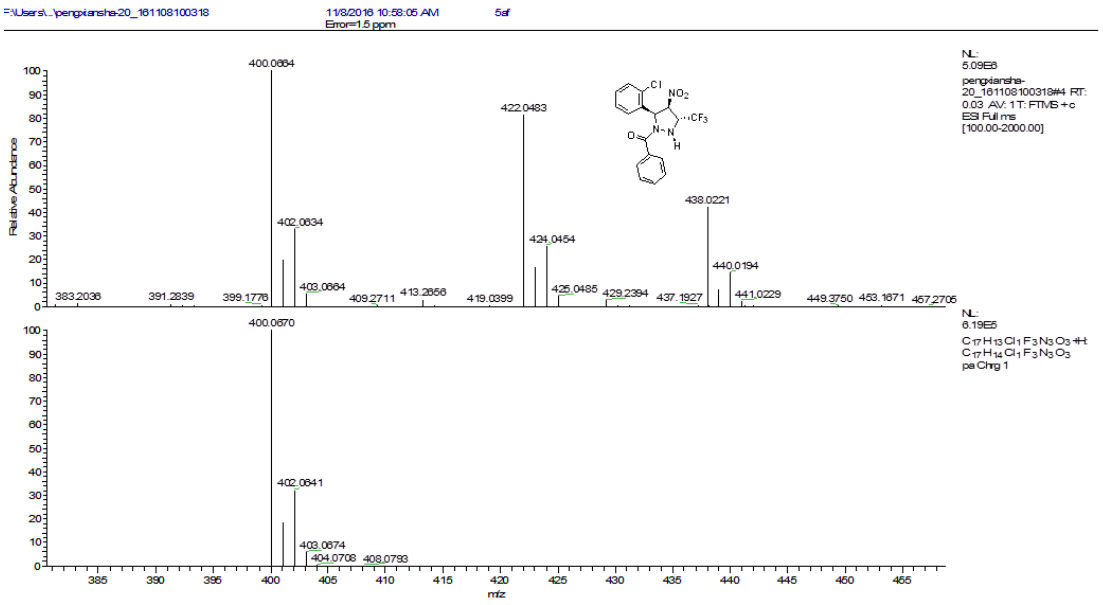
^{13}C NMR copies of compound **3af**:



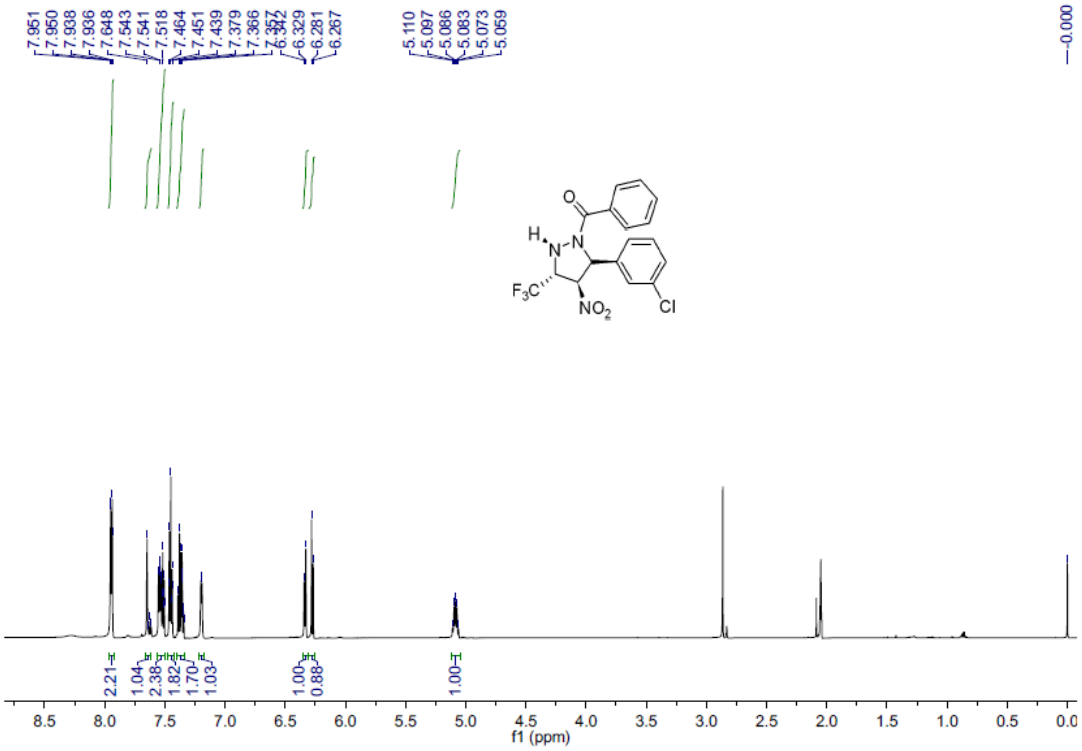
^{19}F NMR copies of compound **3af**:



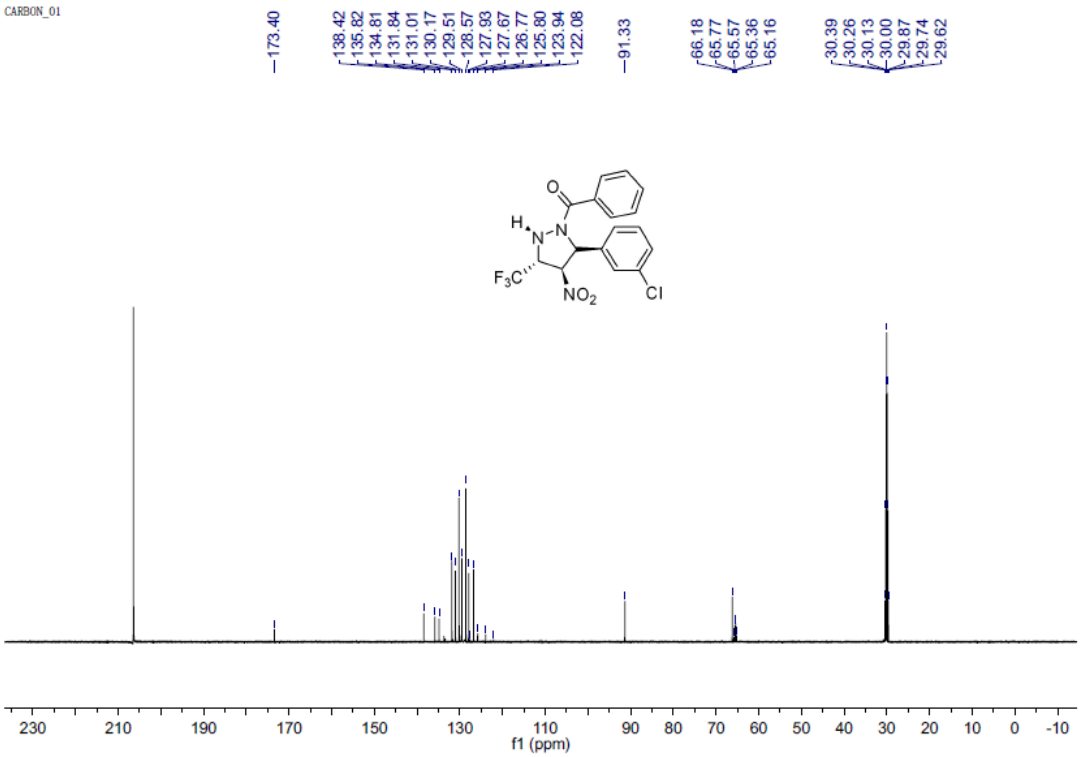
HRMS (ESI) of compound **3af**:



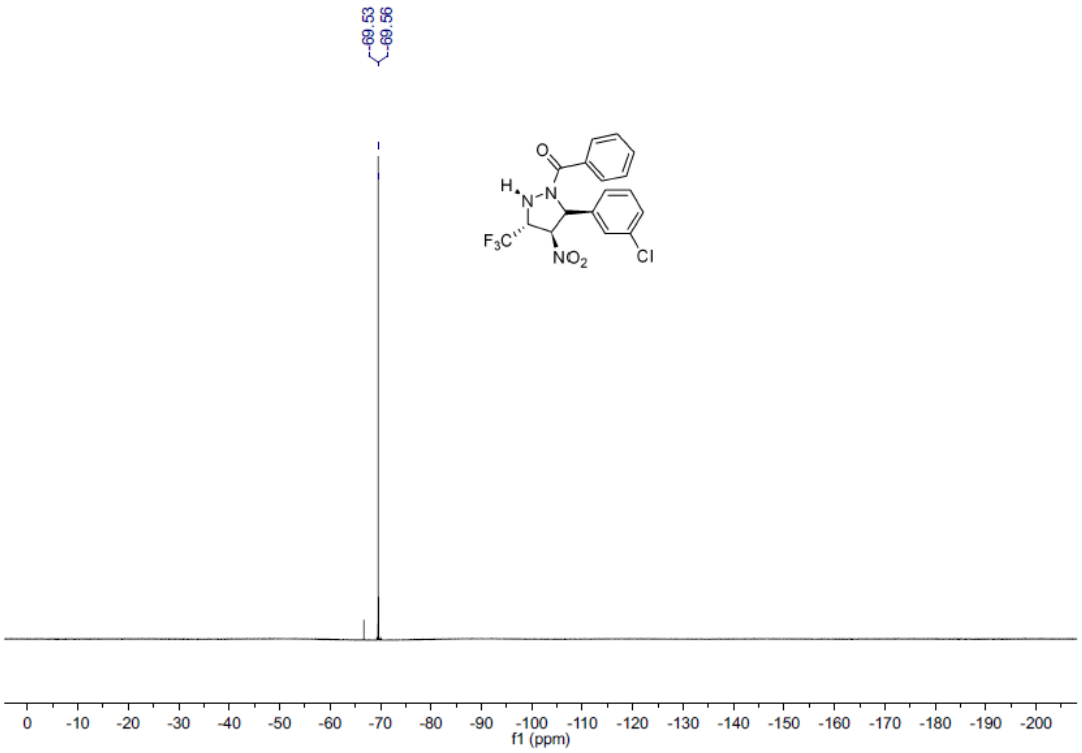
^{1}H NMR copies of compound **3ag**:



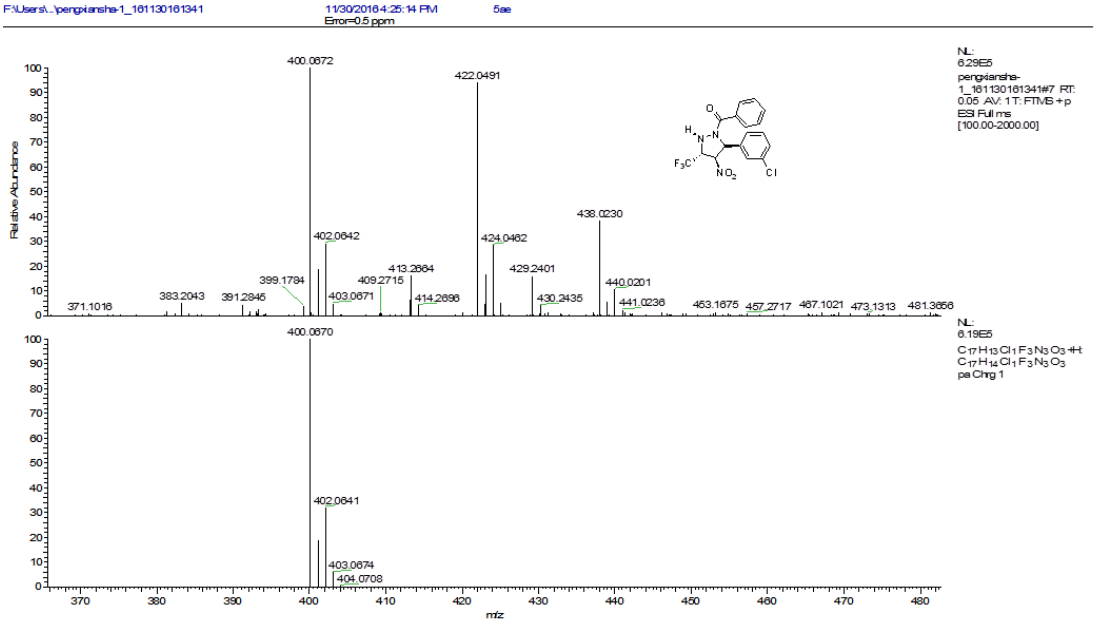
^{13}C NMR copies of compound **3ag**:



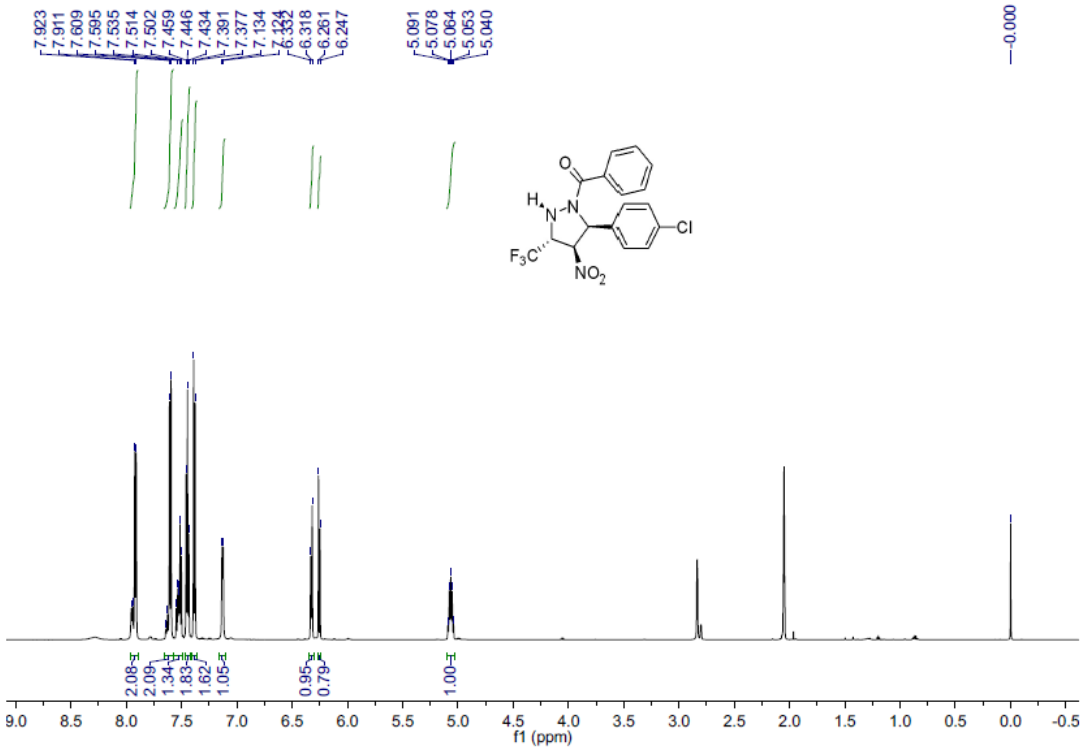
^{19}F NMR copies of compound **3ag**:



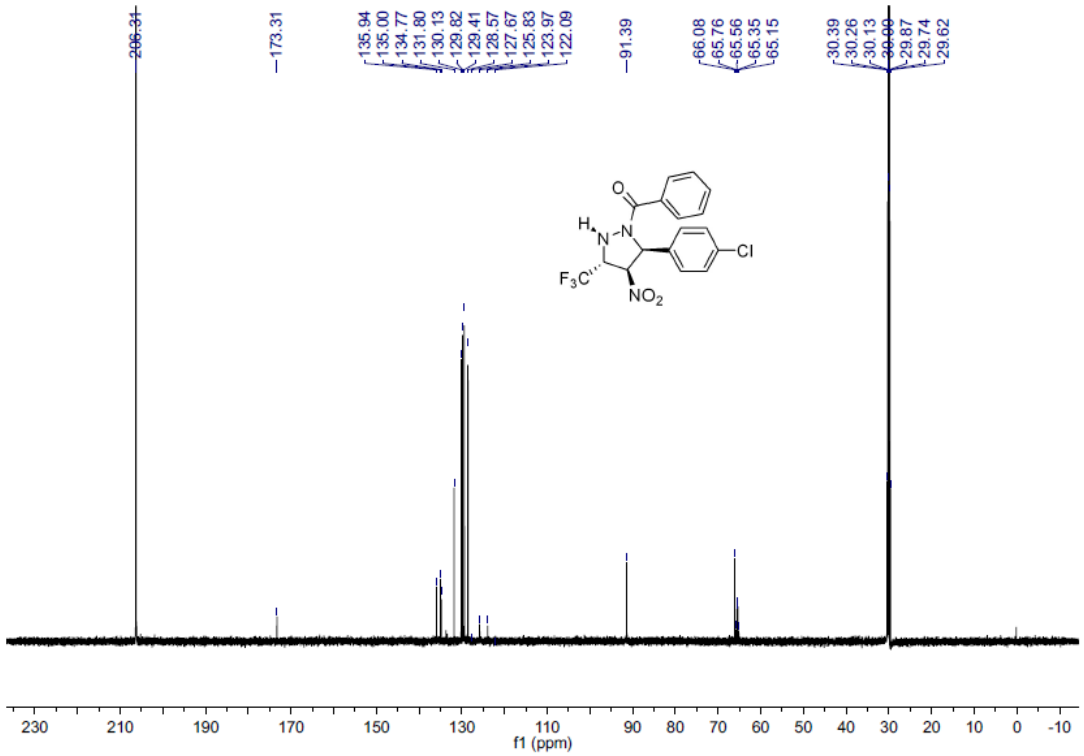
HRMS (ESI) of compound **3ag**:



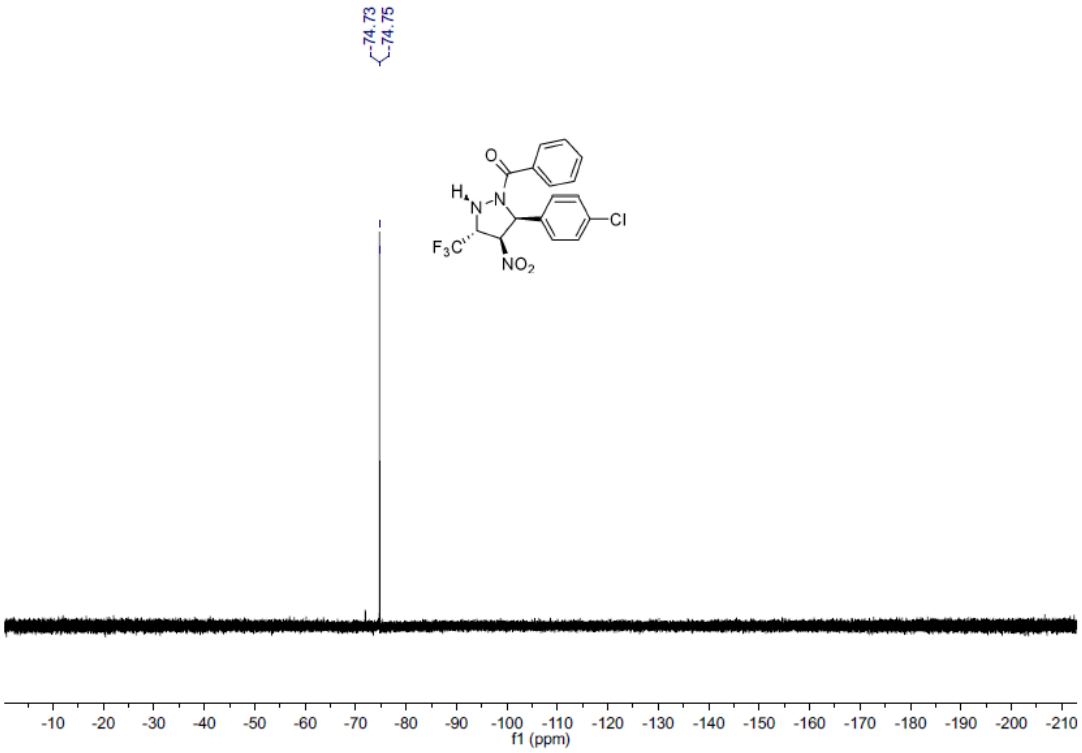
^{1}H NMR copies of compound **3ah**:



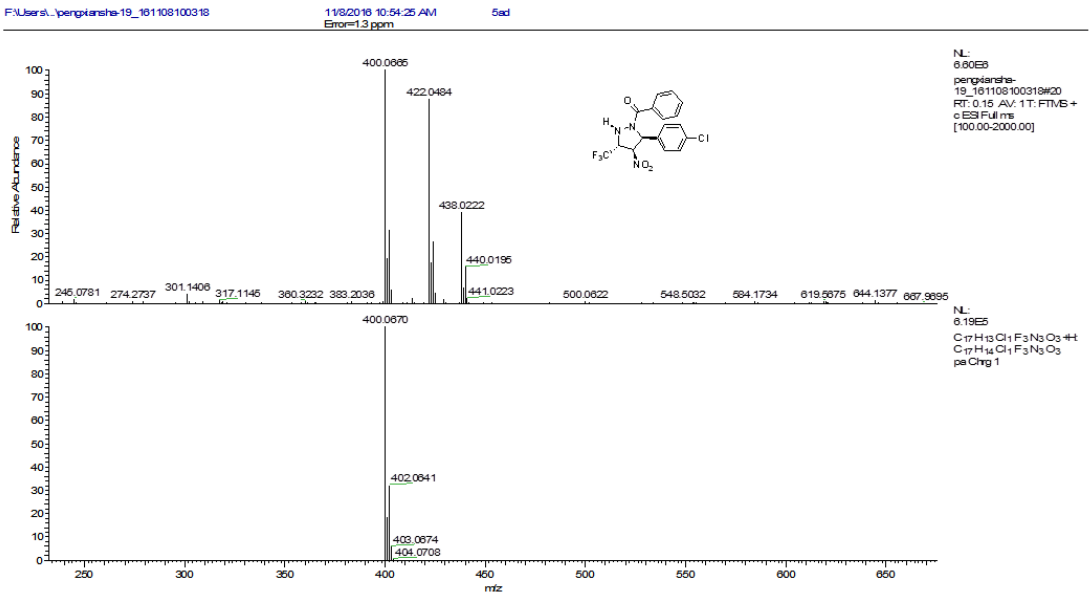
^{13}C NMR copies of compound **3ah**:



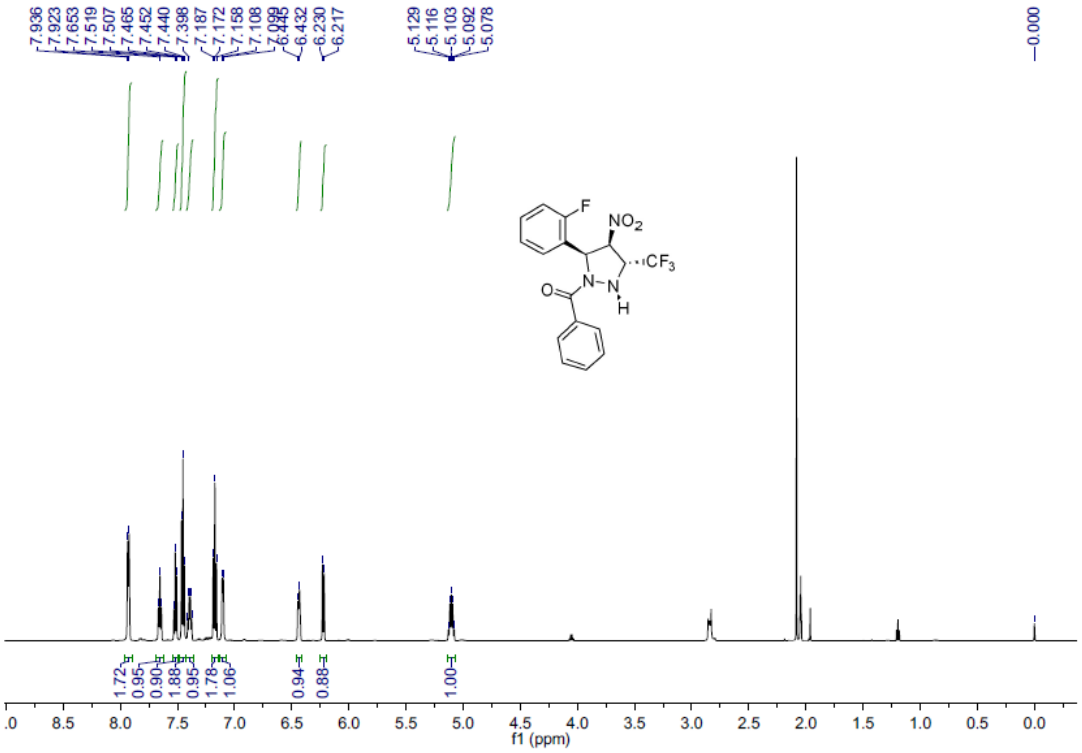
^{19}F NMR copies of compound **3ah**:



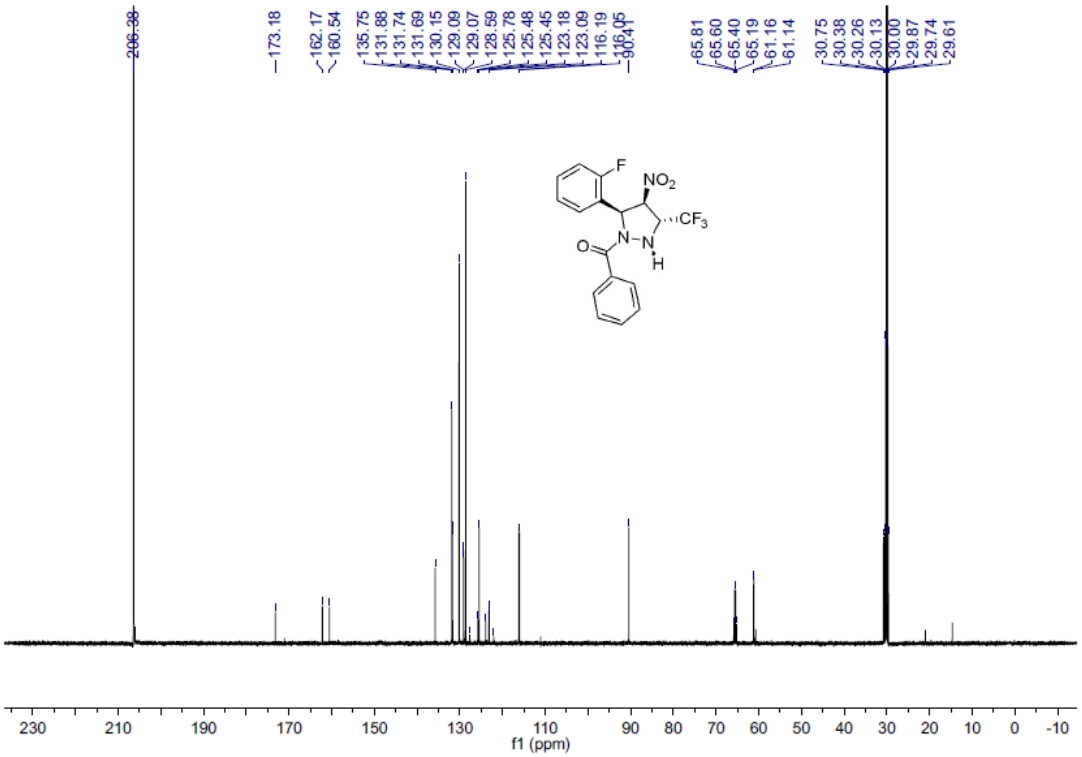
HRMS (ESI) of compound **3ah**:



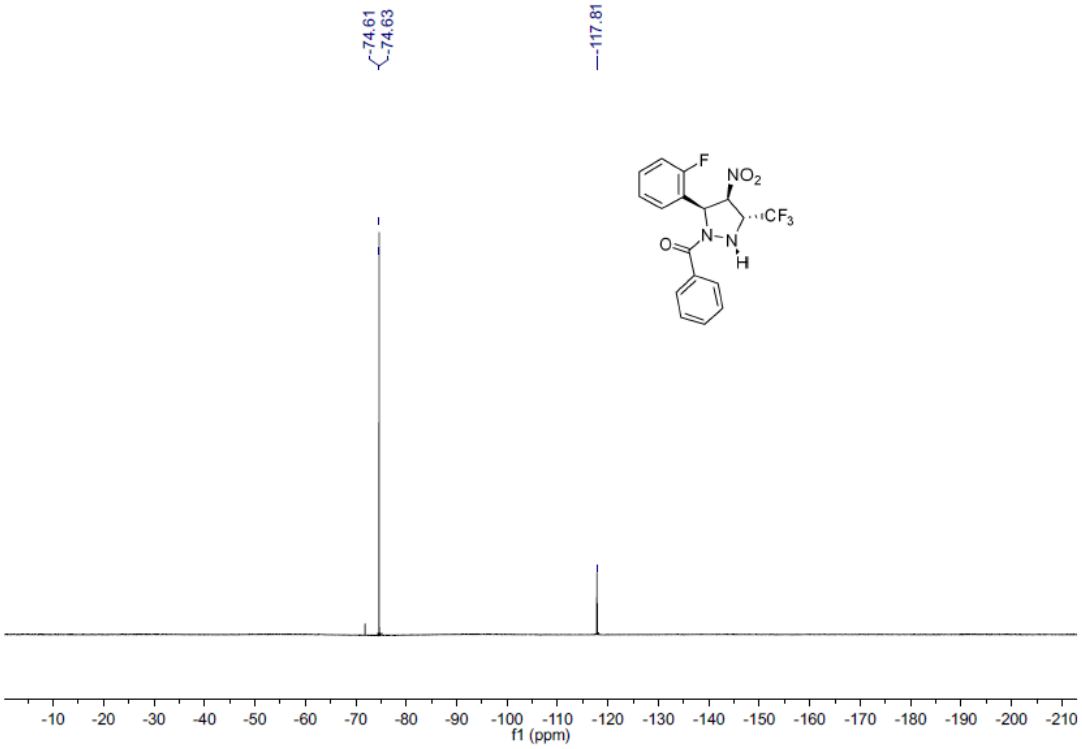
^{1}H NMR copies of compound **3ai**:



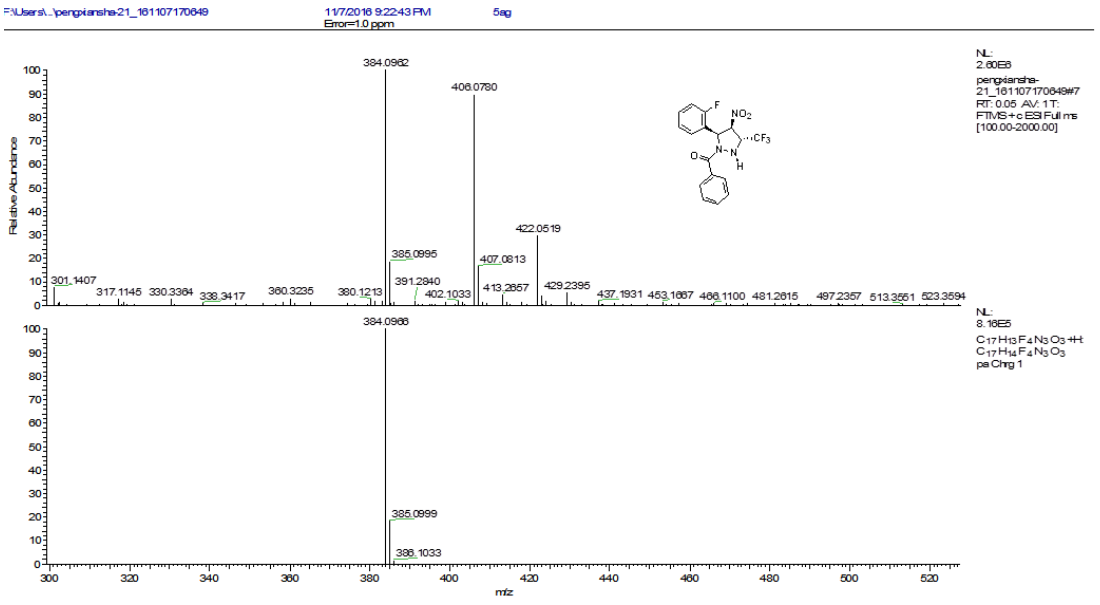
^{13}C NMR copies of compound **3ai**:



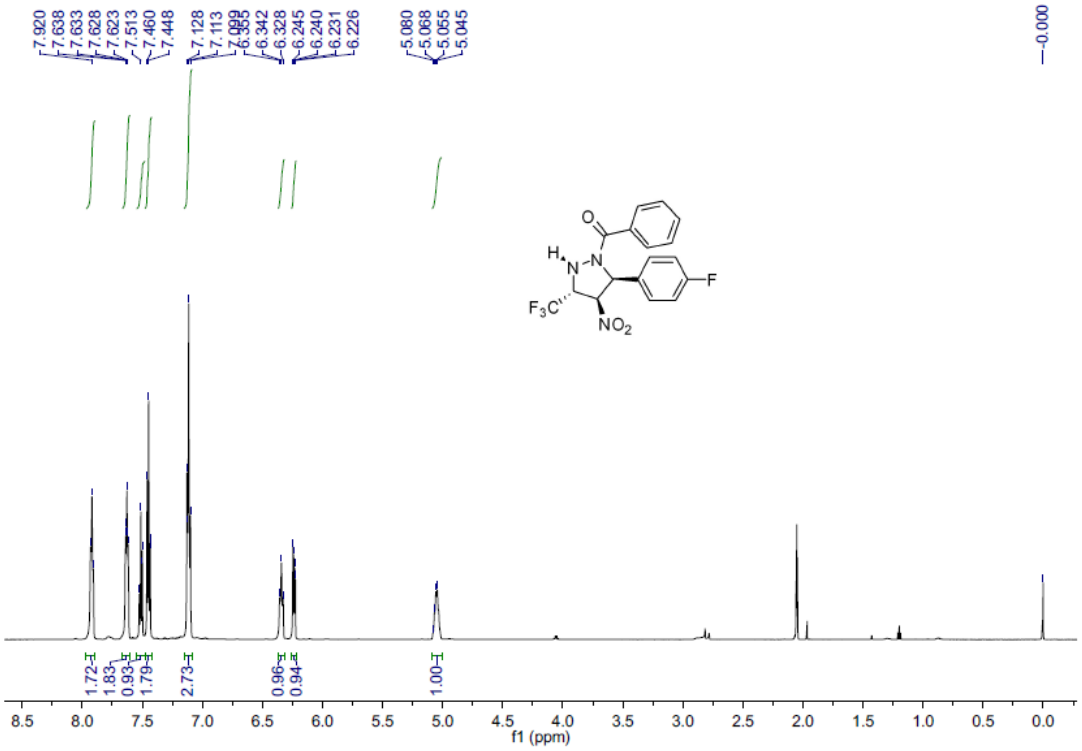
^{19}F NMR copies of compound **3ai**:



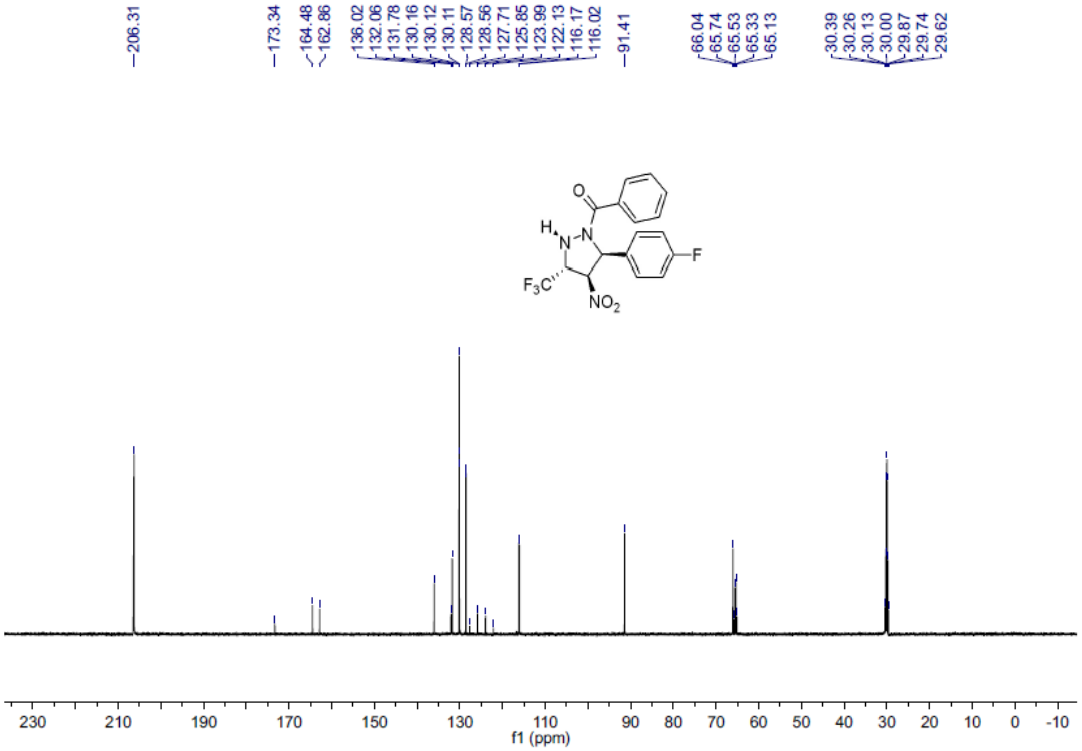
HRMS (ESI) of compound **3ai**:



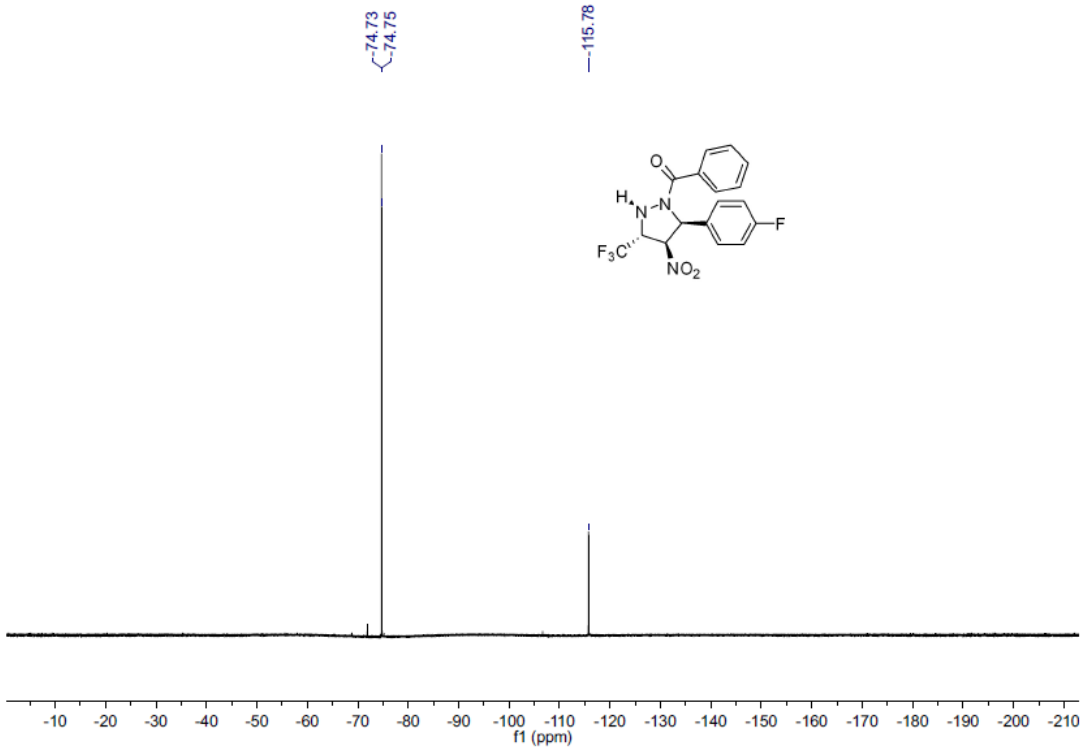
^{1}H NMR copies of compound **3aj**:



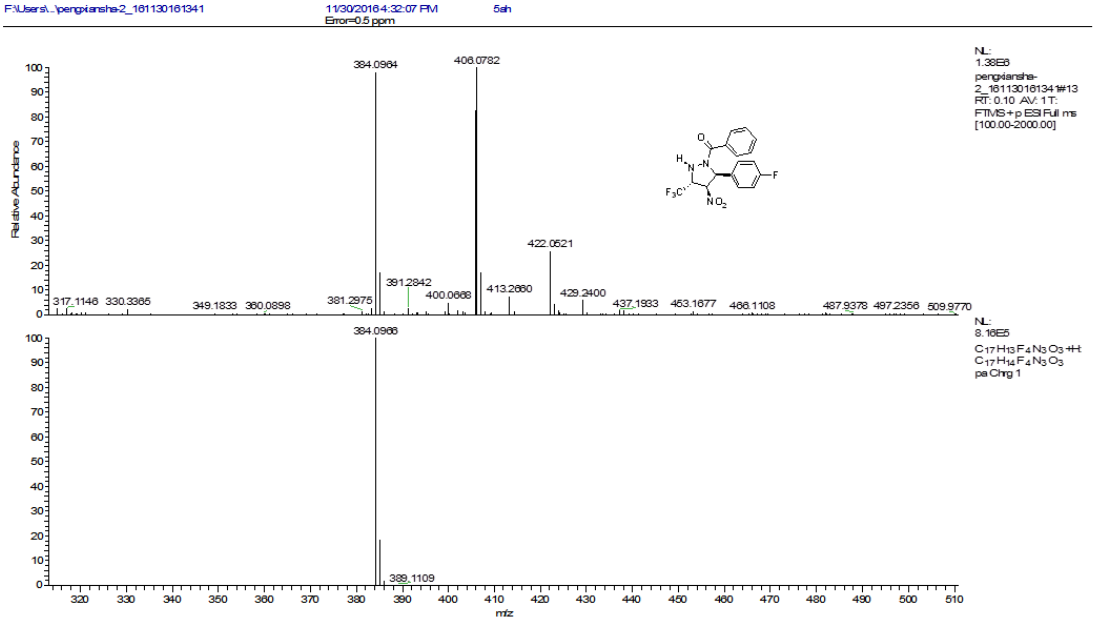
^{13}C NMR copies of compound **3aj**:



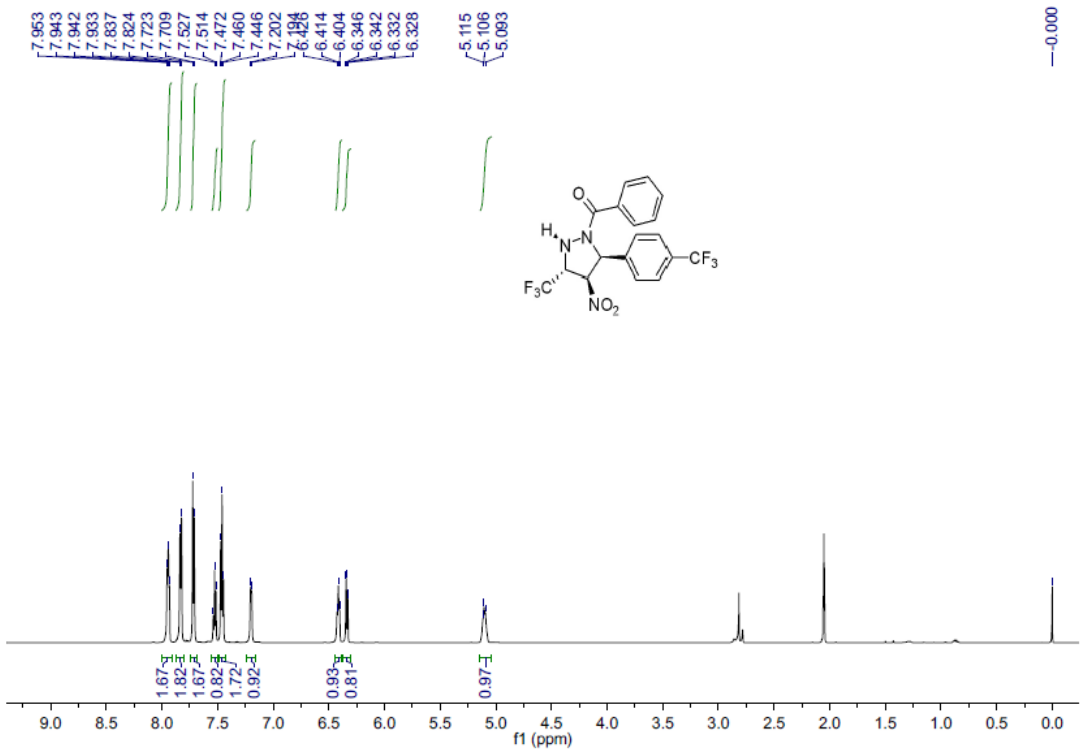
^{19}F NMR copies of compound **3aj**:



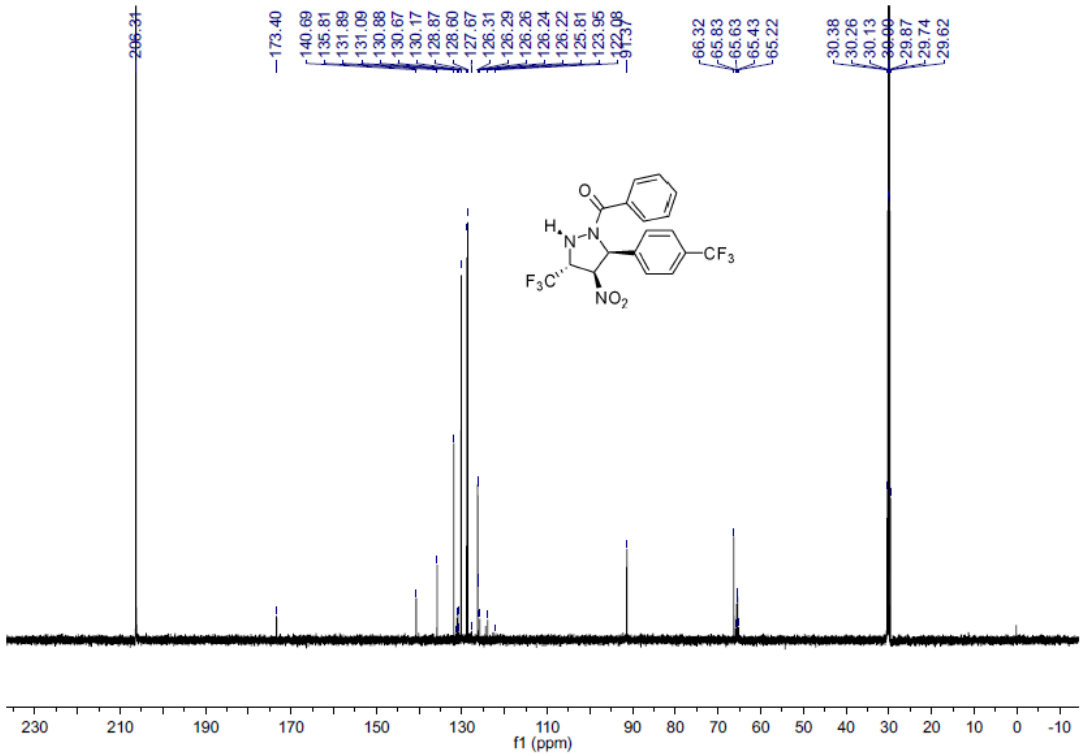
HRMS (ESI) of compound **3aj**:

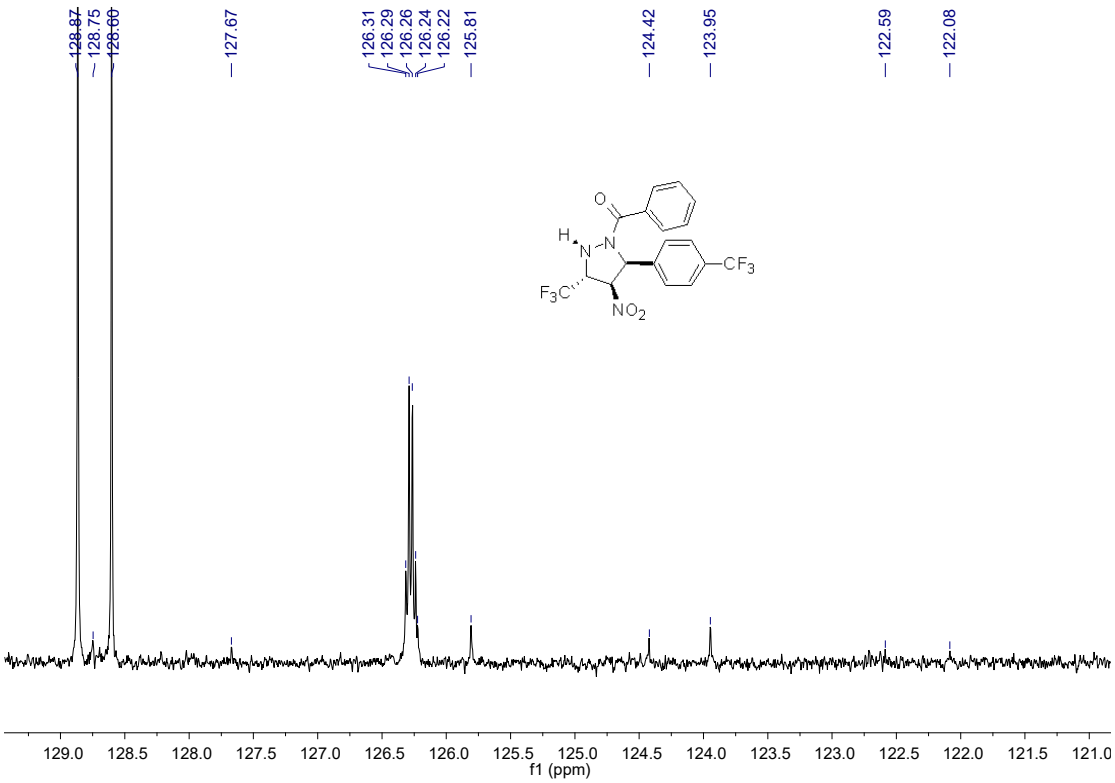


^{1}H NMR copies of compound **3ak**:

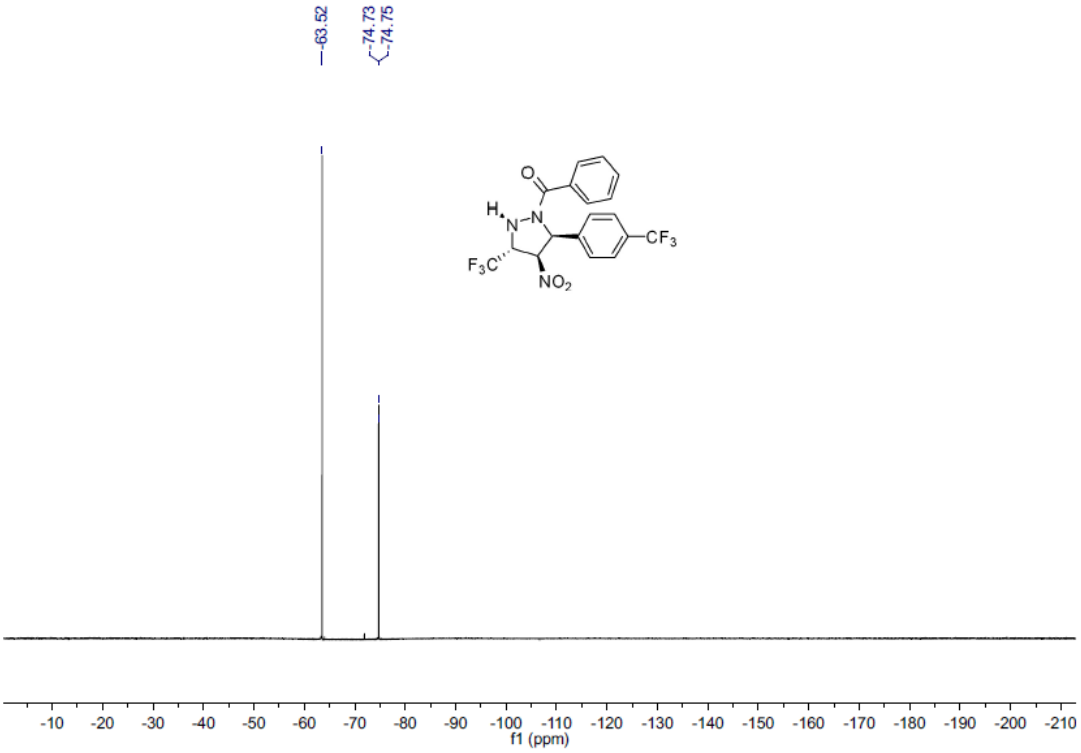


^{13}C NMR copies of compound **3ak**:

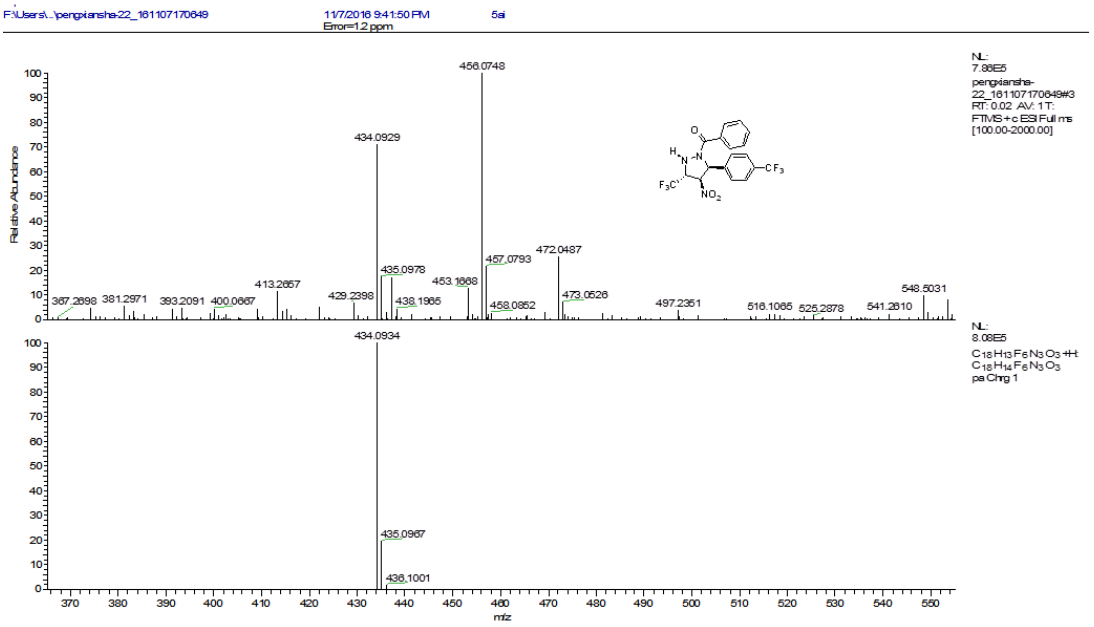




^{19}F NMR copies of compound **3ak**:



HRMS (ESI) of compound **3ak**:


F:\Users\..\pengxiansha-22_161107170649
11/7/2016 9:41:50 PM
5ai
Error=1.2 ppm
NL:
7.88E5
pengxiansha-22_161107170649#3 RT: 0.02 AV: 1 T: FTMS + c ESI Full ms [100.00-2000.00]
456.0748
434.0929
435.0978
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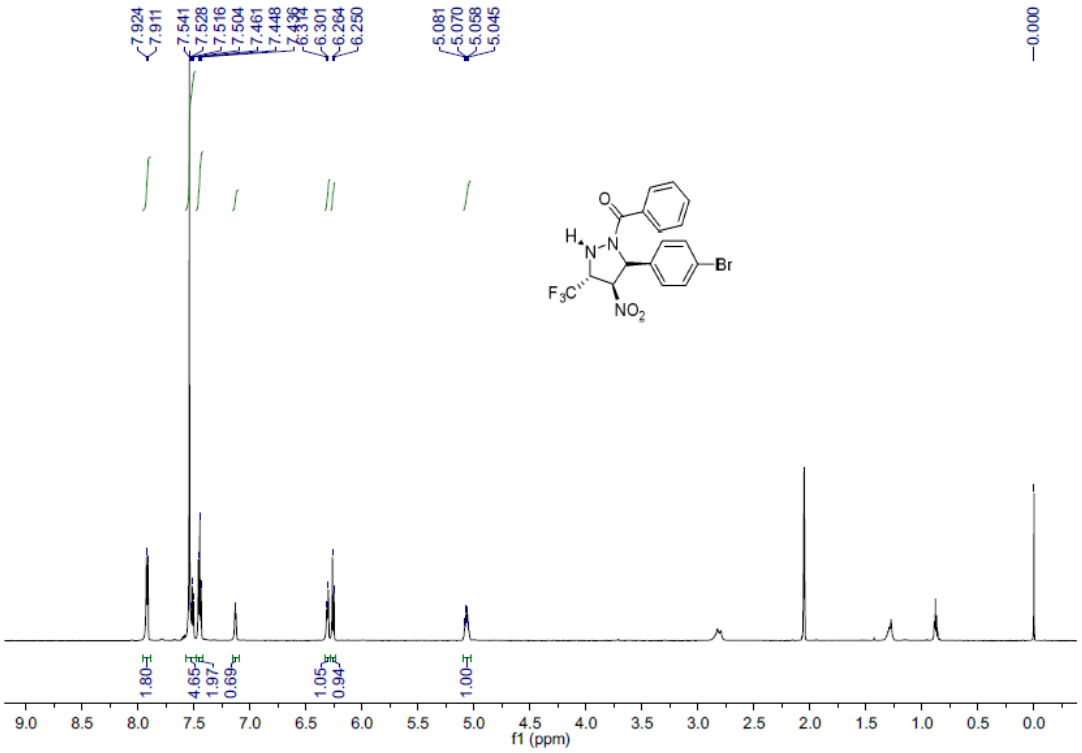
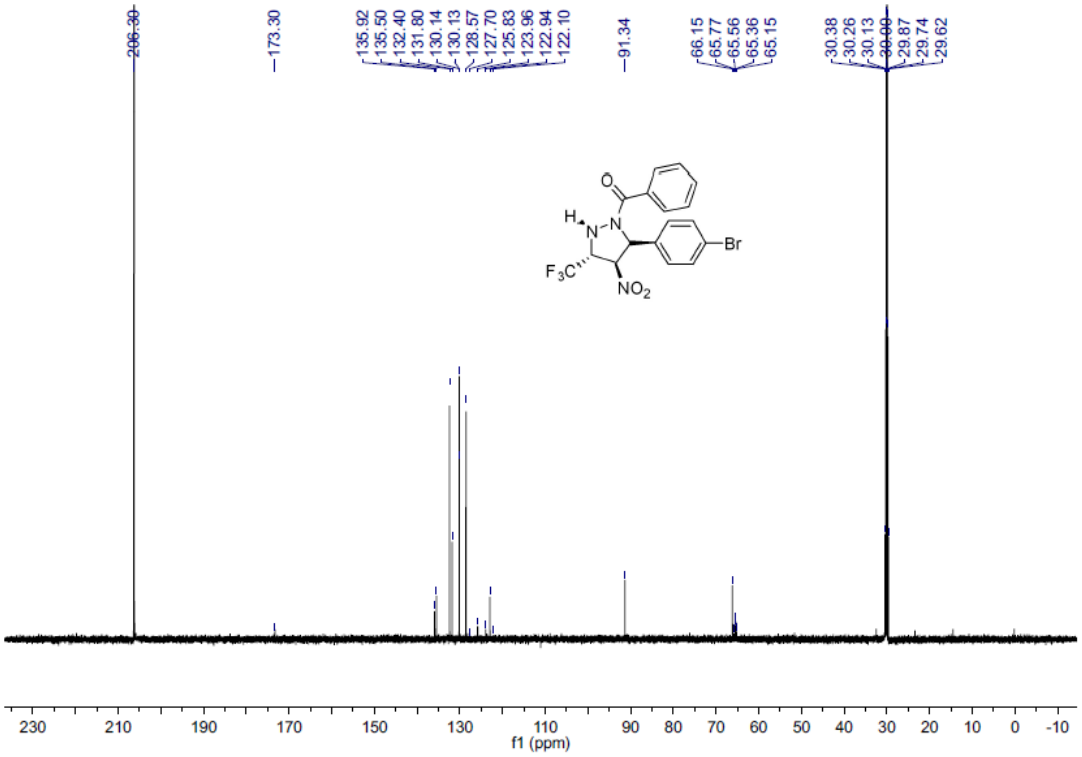
472.0487
453.1868
413.2657
429.2398
438.1965
458.0852
473.0526
497.2351
516.1065
525.2878
541.2610
548.5031
387.2698
381.2971
393.2091
400.0667
NL:
8.08E5
C18H13F6N3O3+H
C18H14F6N3O3
pa Chrg 1
434.0934
435.0967
436.1001
Relative Abundance
m/z

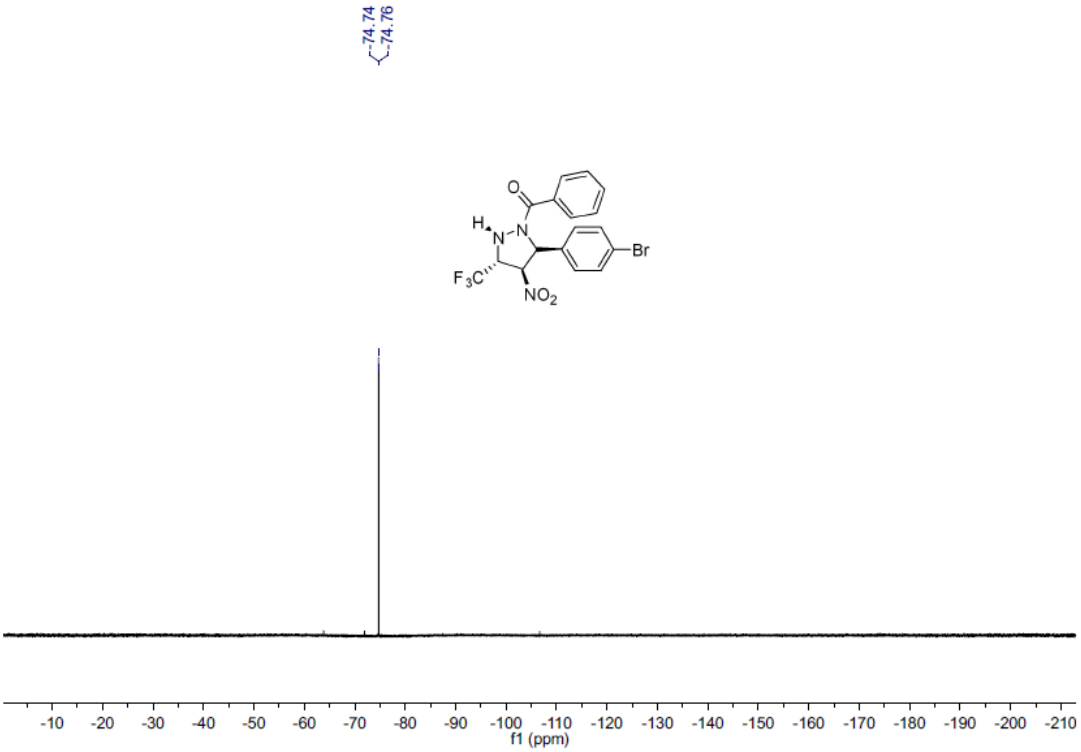
^{1}H NMR copies of compound **3al**:



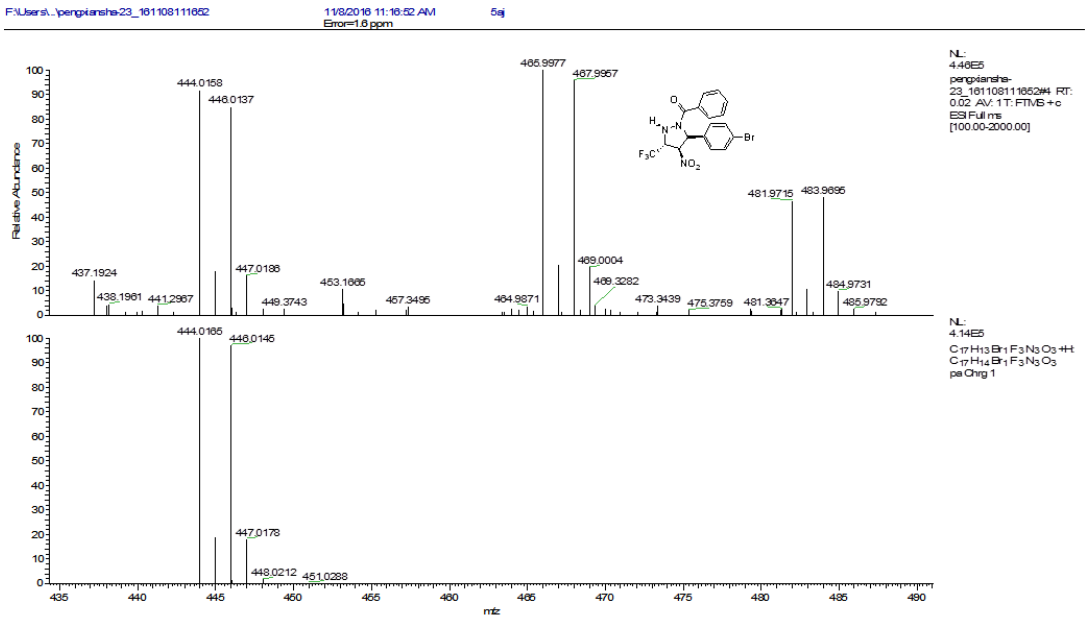
^{13}C NMR copies of compound **3al**:



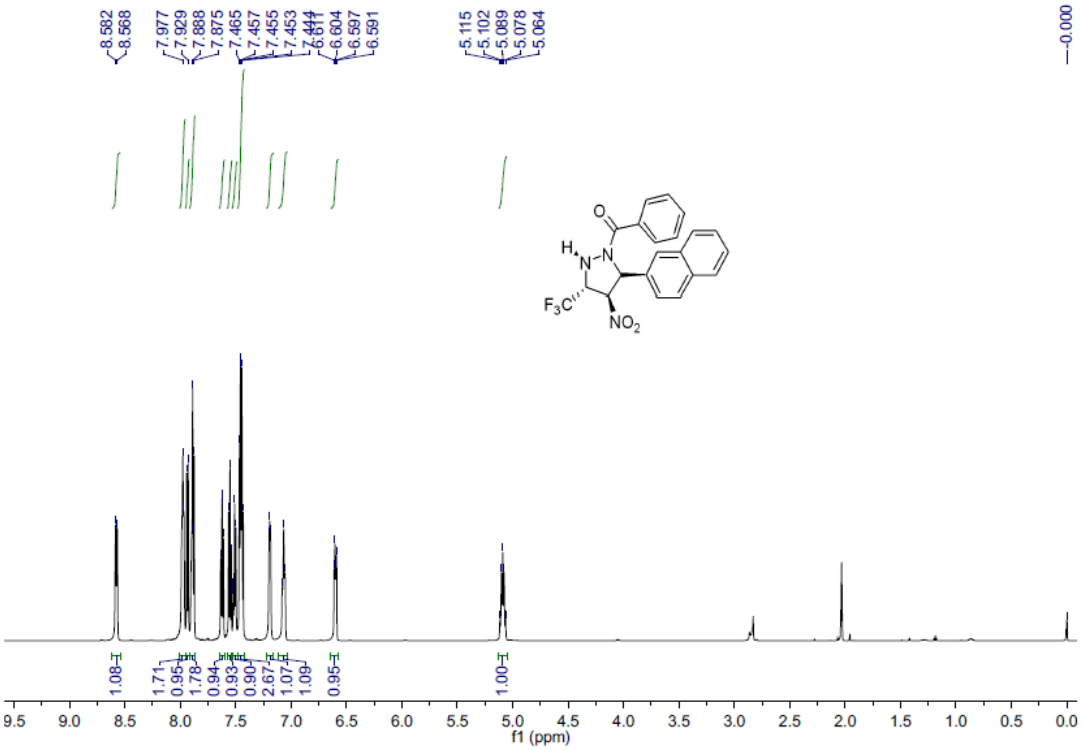
^{19}F NMR copies of compound **3al**:



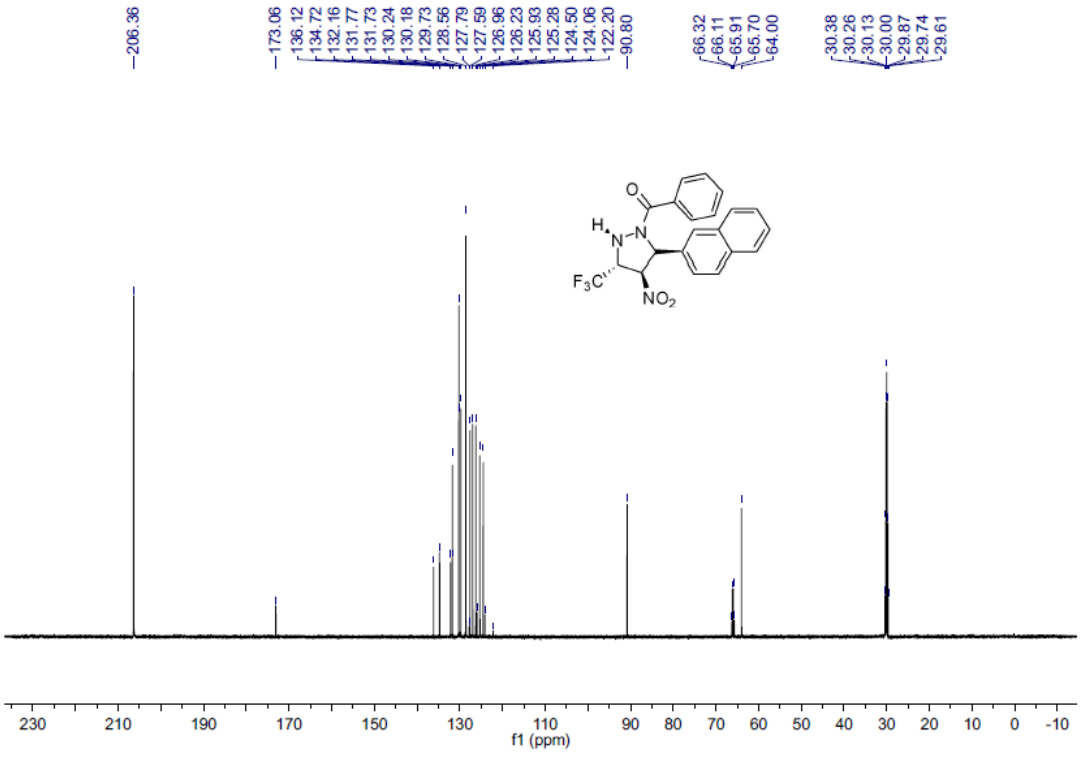
HRMS (ESI) of compound **3al**:



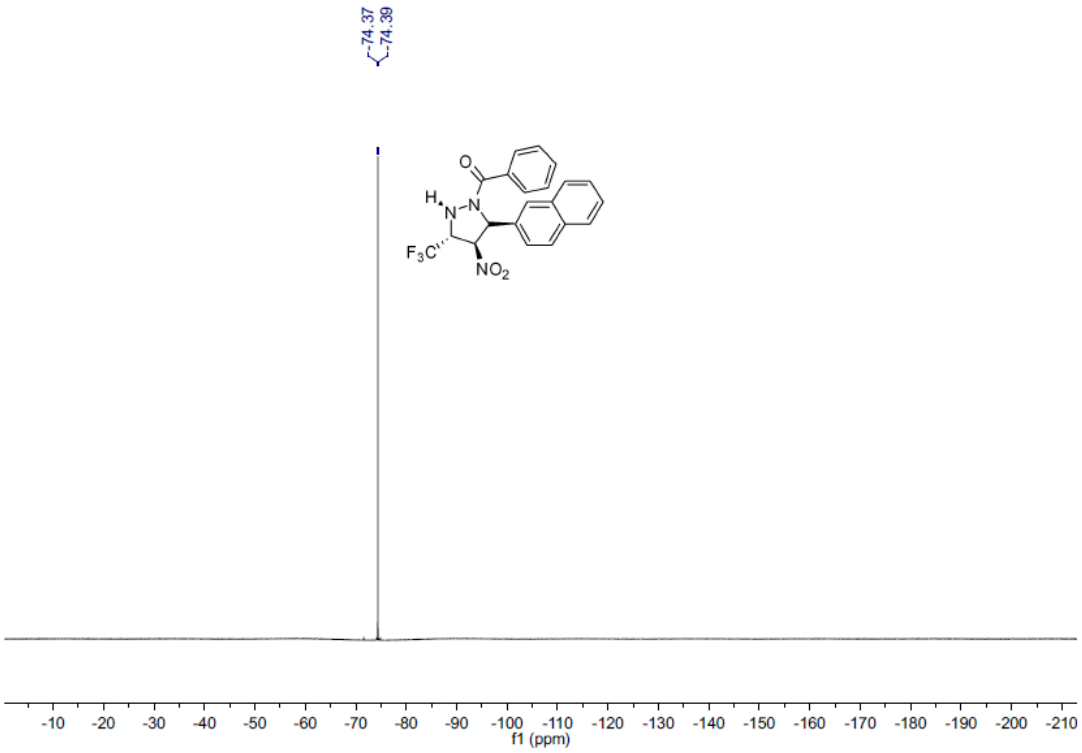
^{1}H NMR copies of compound **3am**:



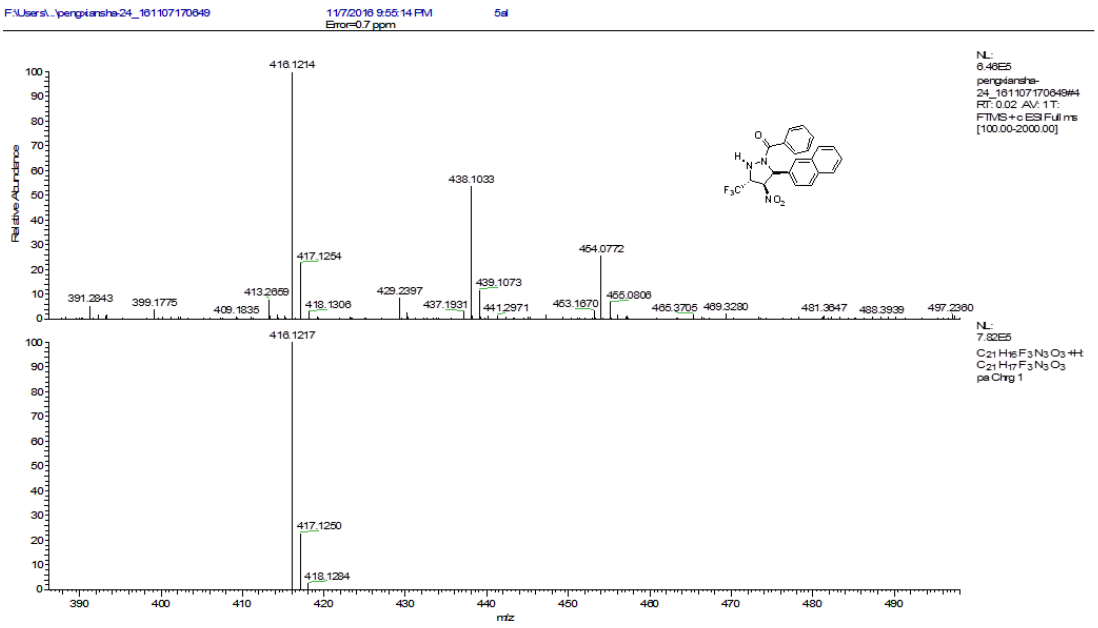
^{13}C NMR copies of compound **3am**:



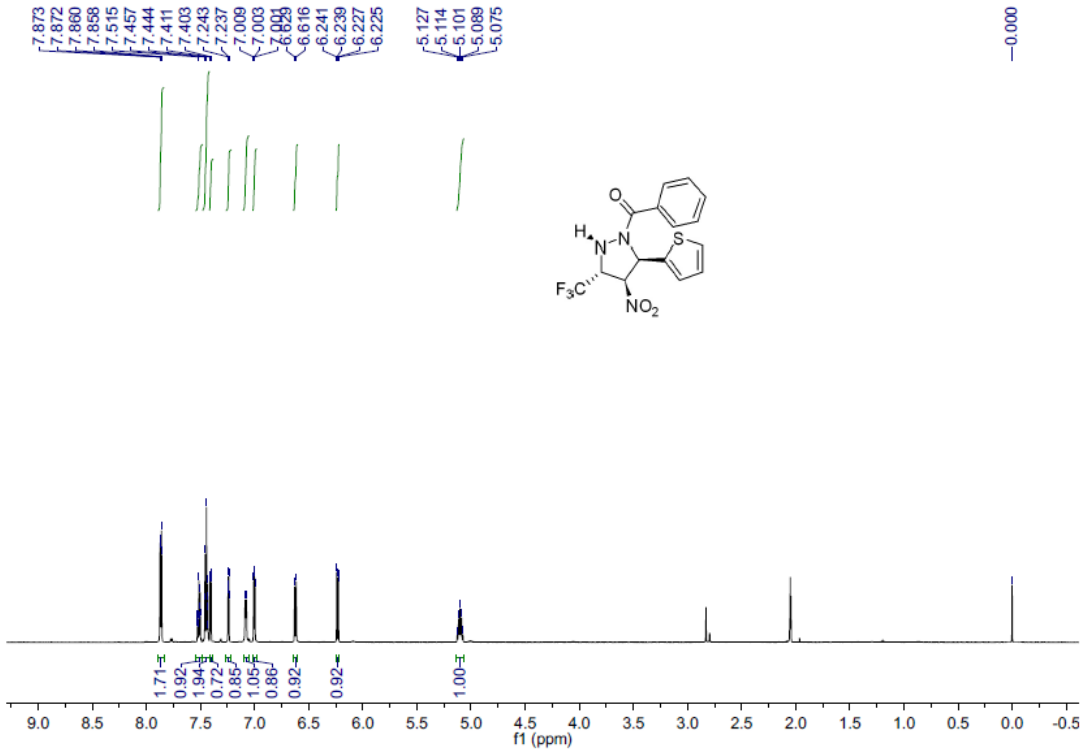
^{19}F NMR copies of compound **3am**:



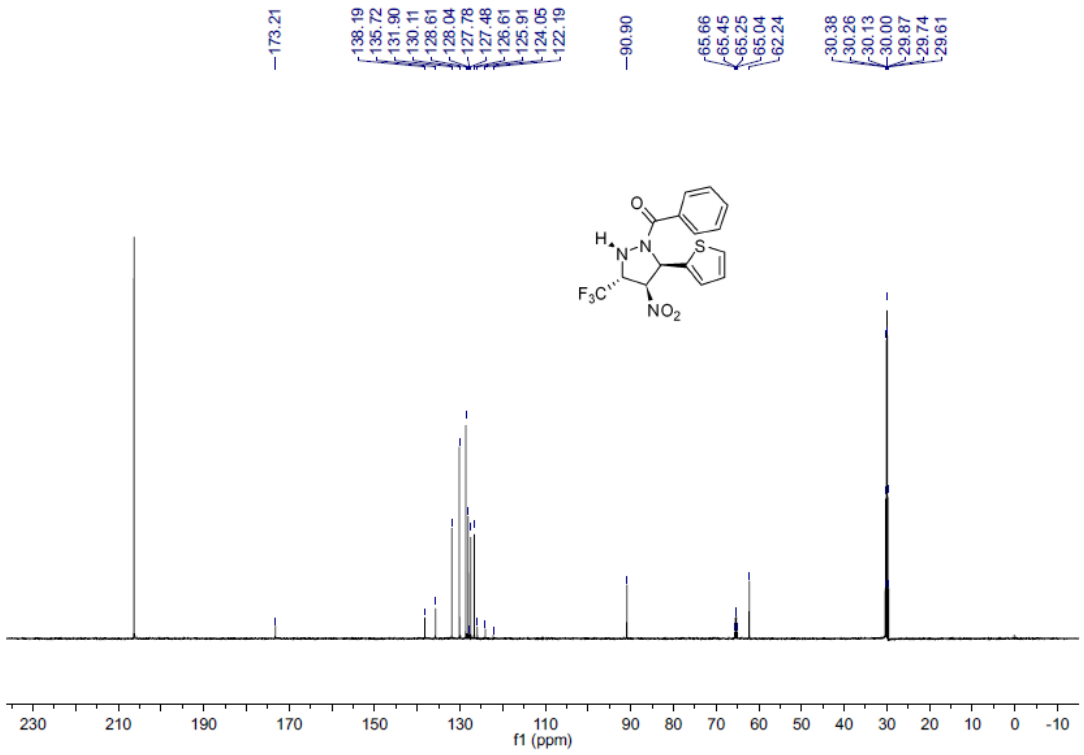
HRMS (ESI) of compound **3am**:



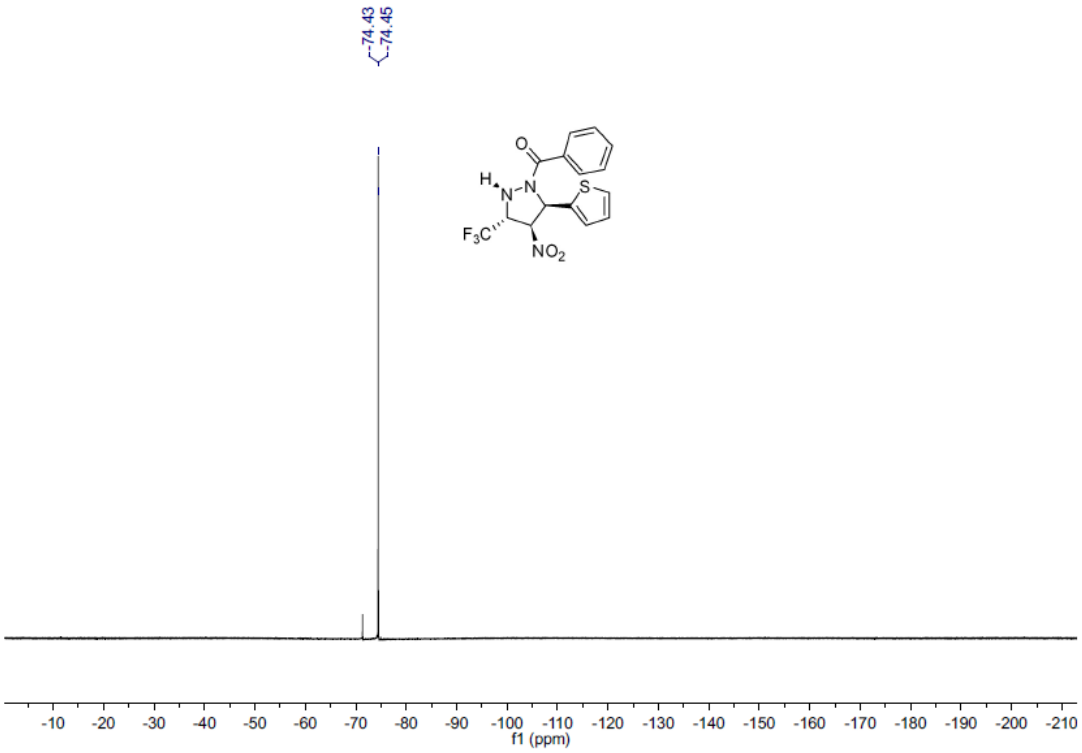
[1]H NMR copies of compound **3an**:



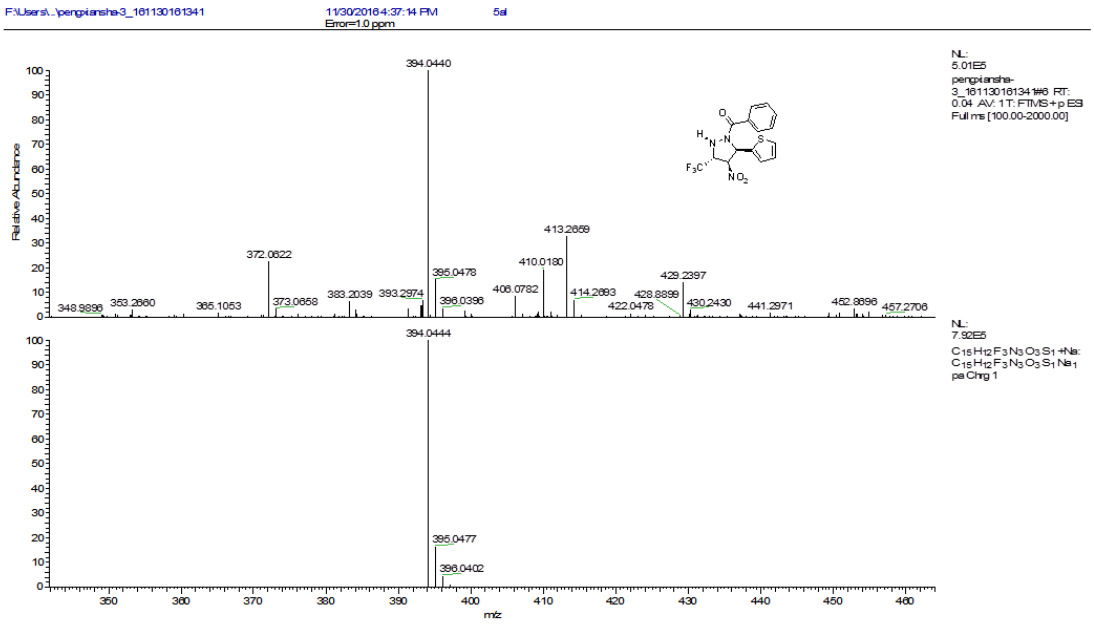
[13]C NMR copies of compound **3an**:



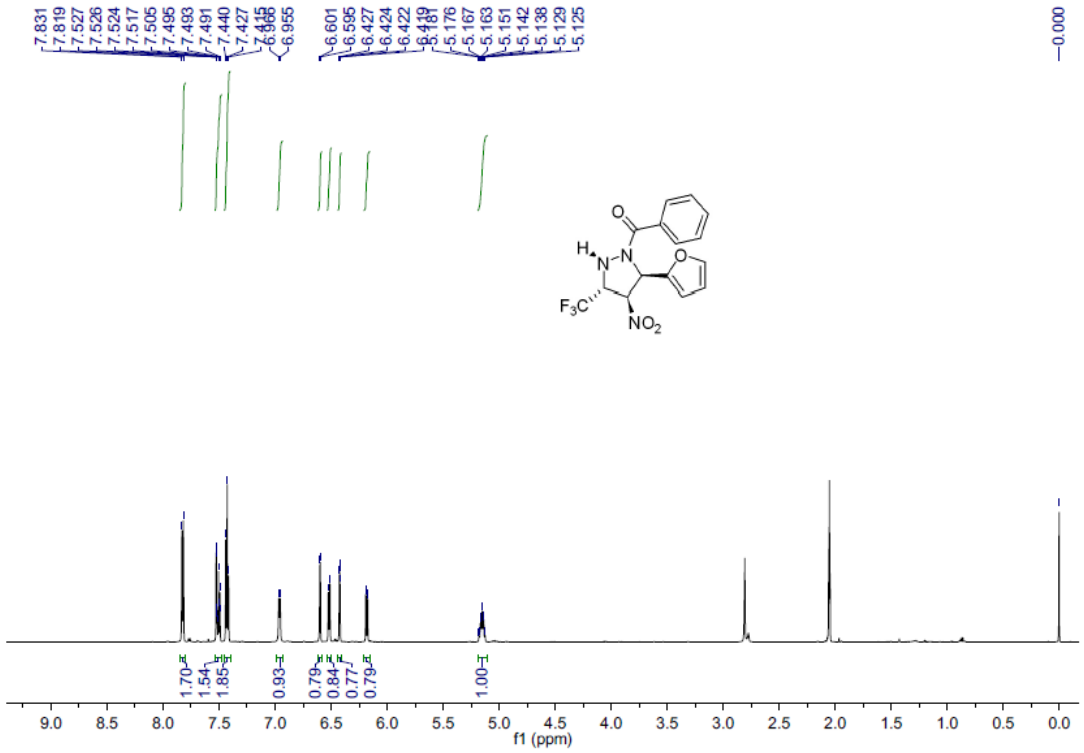
^{19}F NMR copies of compound **3an**:



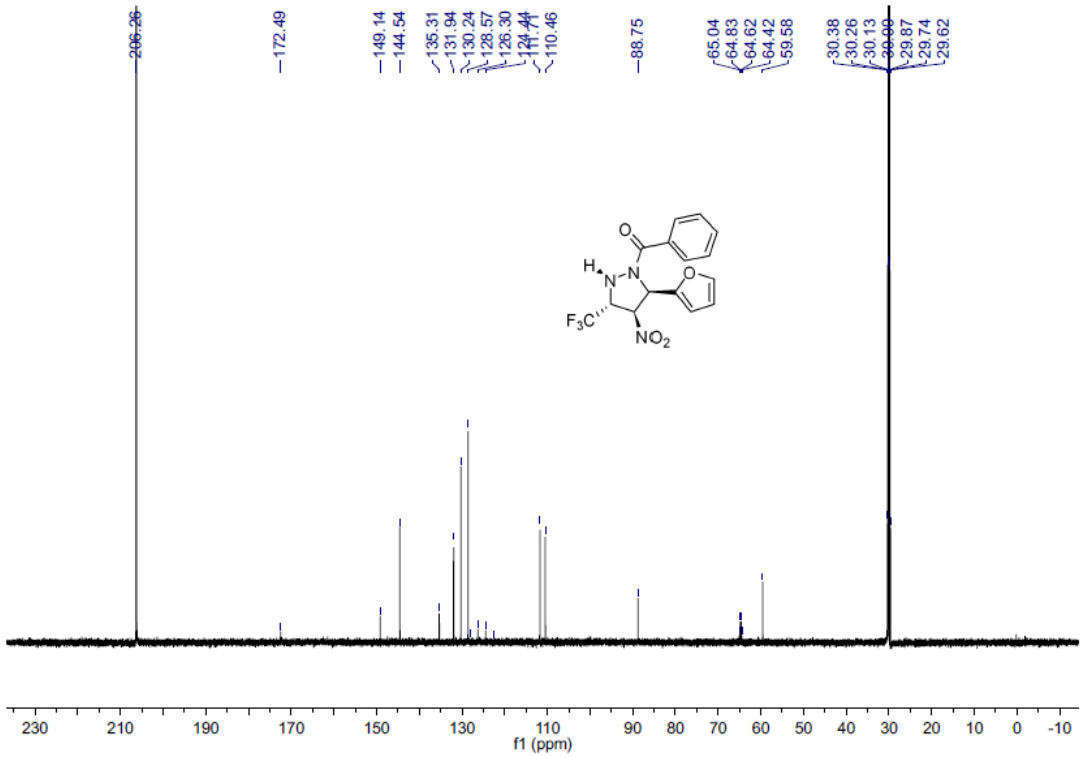
HRMS (ESI) of compound **3an**:



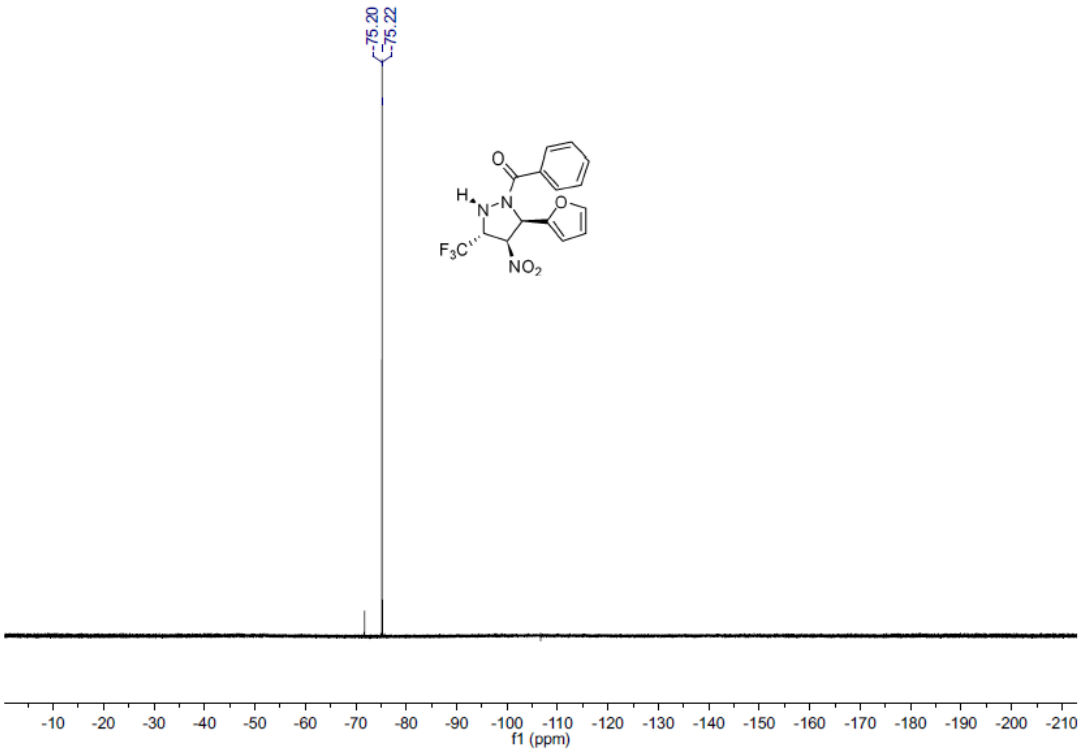
^{1}H NMR copies of compound **3ao**:



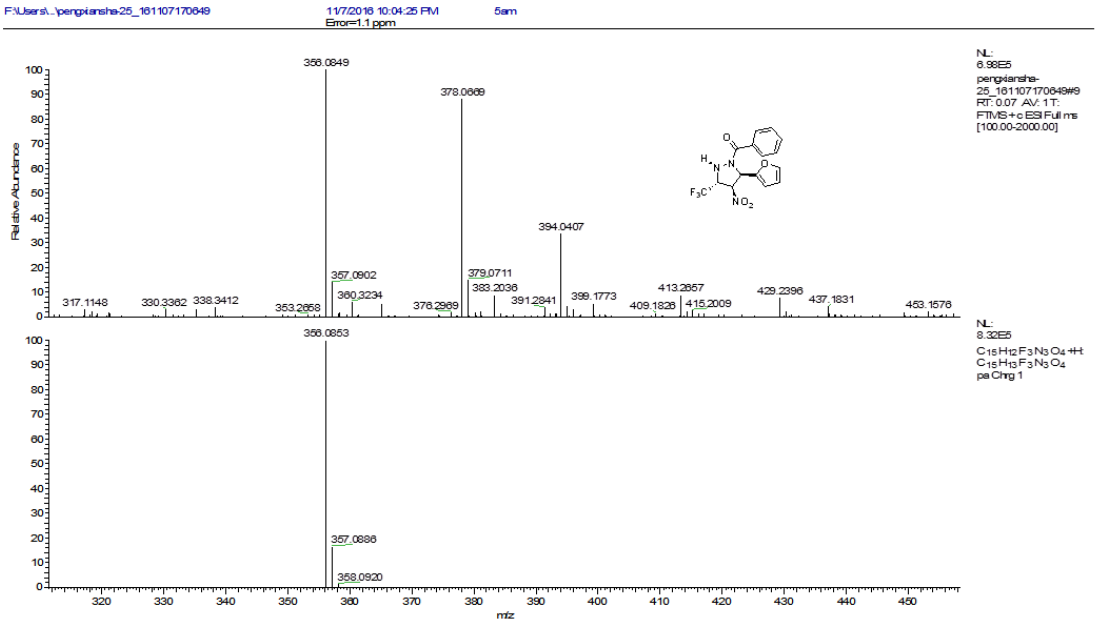
^{13}C NMR copies of compound **3ao**:



^{19}F NMR copies of compound **3ao**:

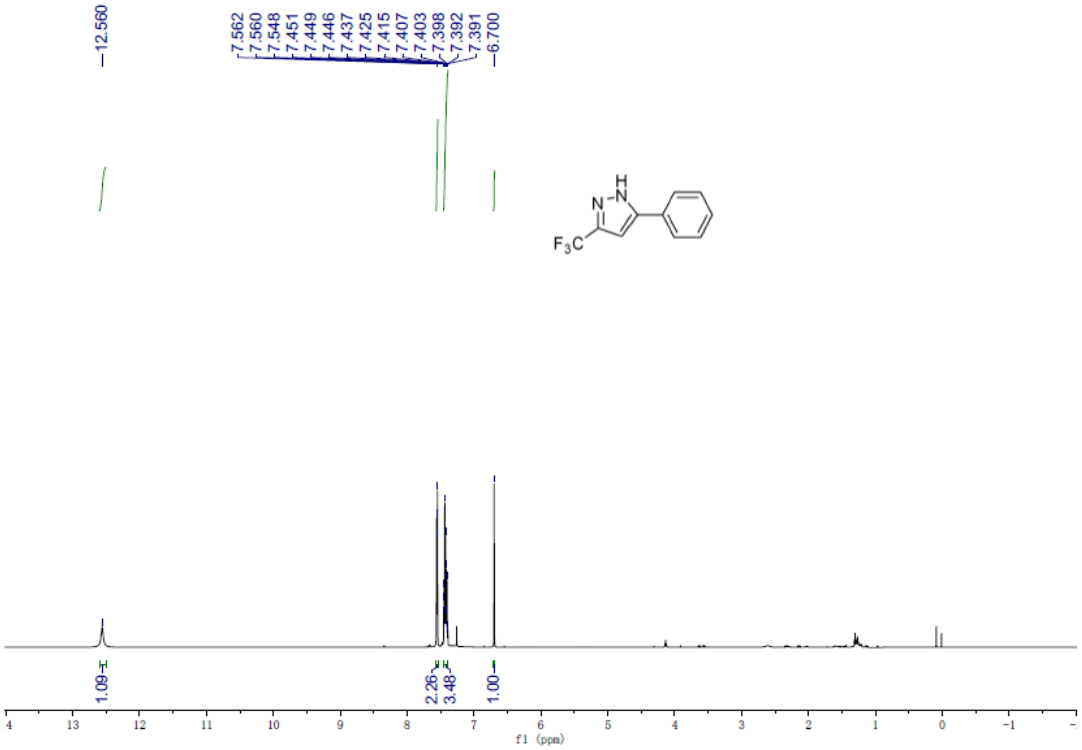


HRMS (ESI) of compound **3ao**:

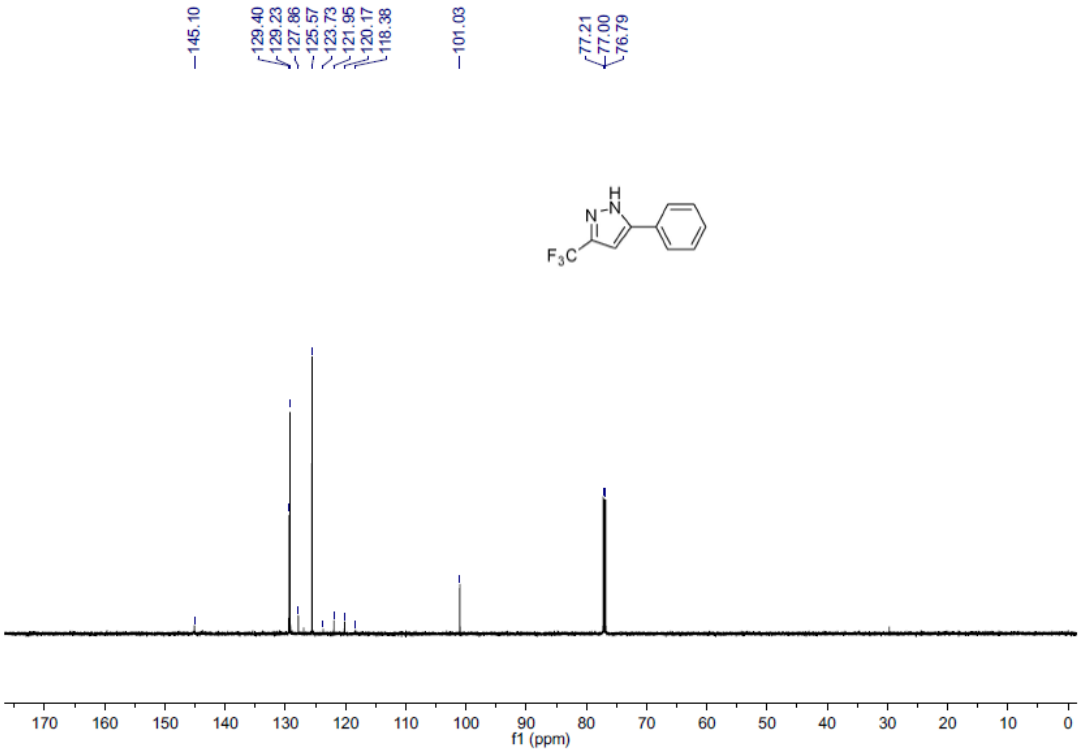


8 NMR, HRMS copies of compounds 4a-4d

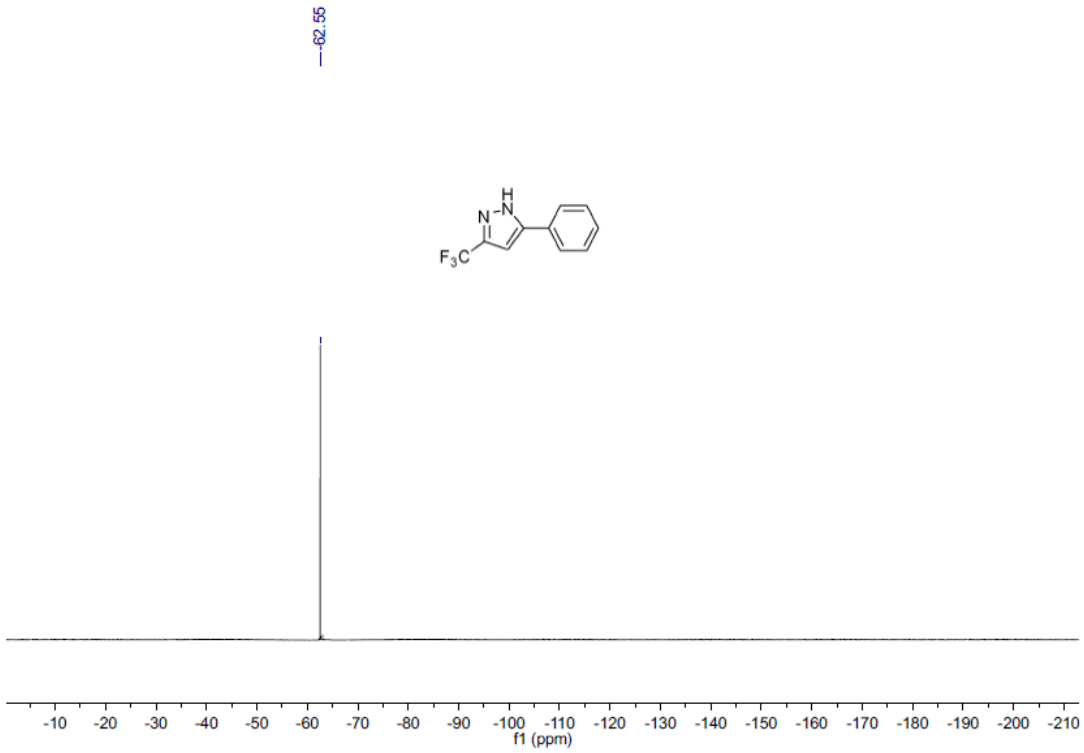
^{1}H NMR copies of compound **4a**:



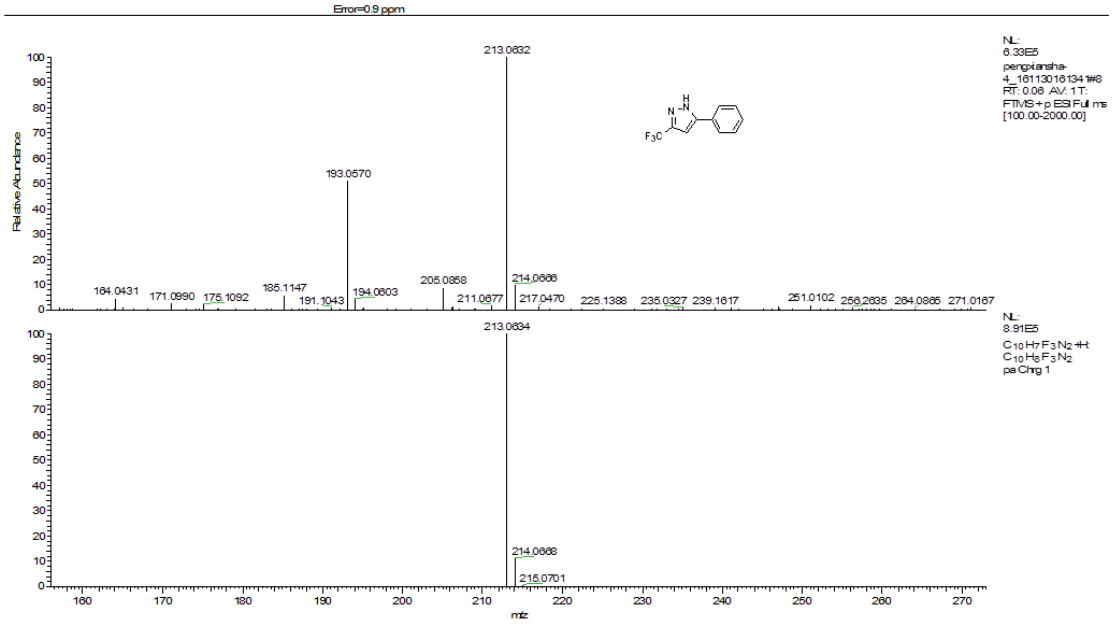
^{13}C NMR copies of compound **4a**:



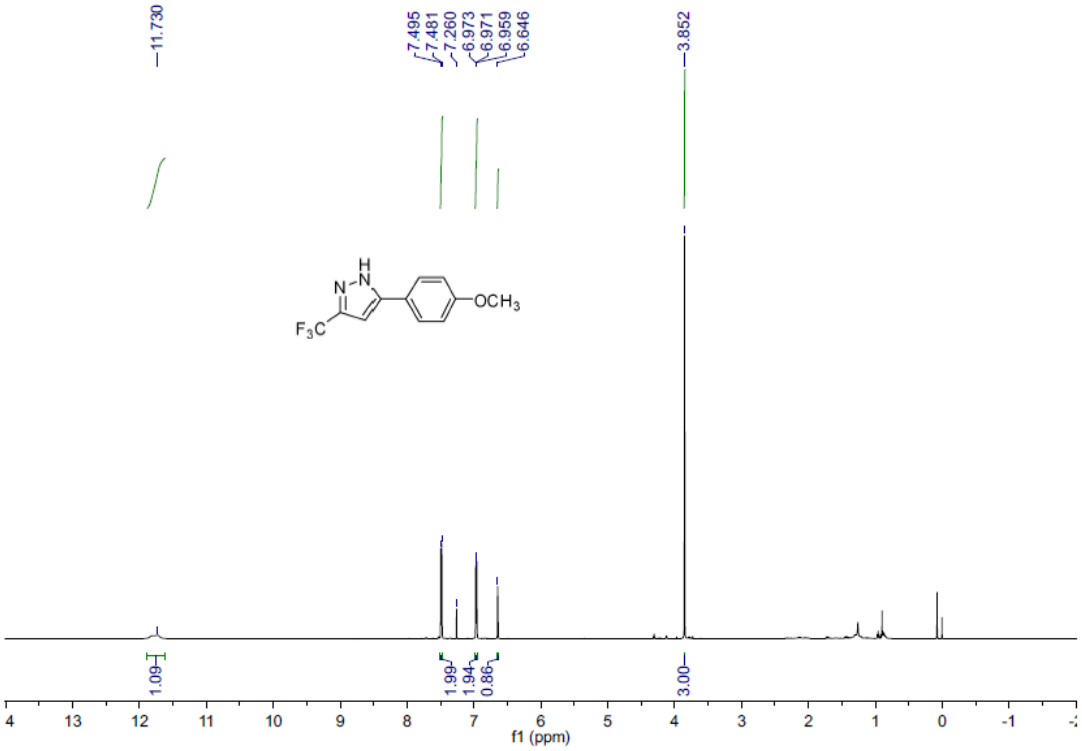
^{19}F NMR copies of compound **4a**:



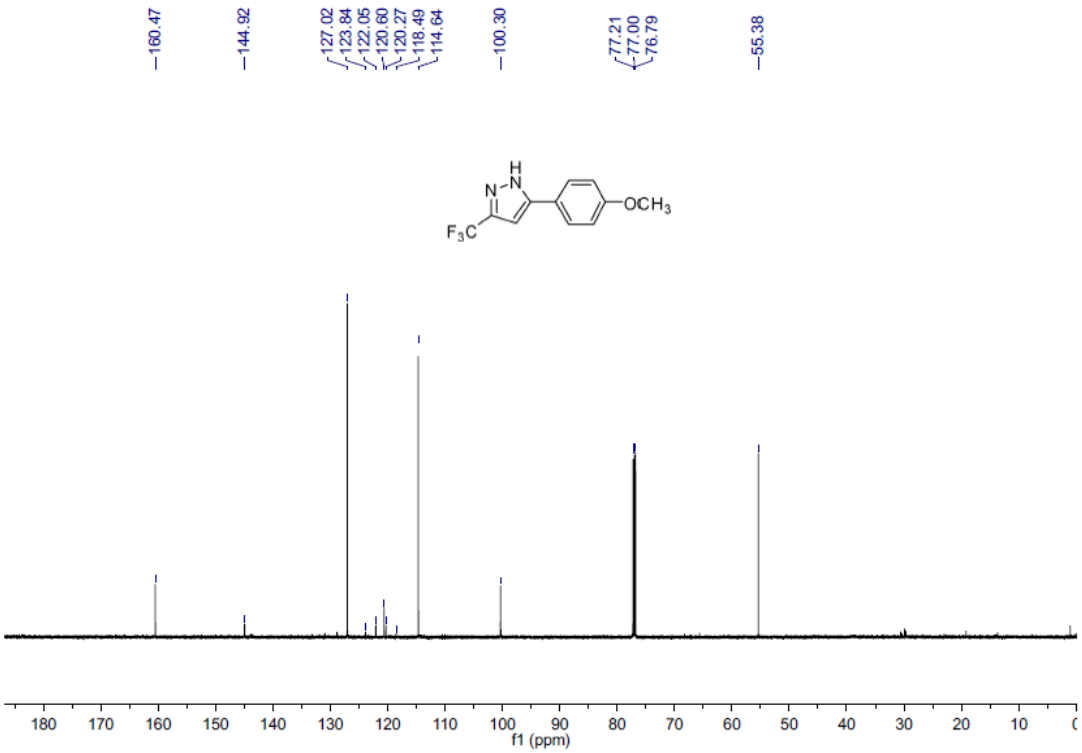
HRMS (ESI) of compound **4a**:



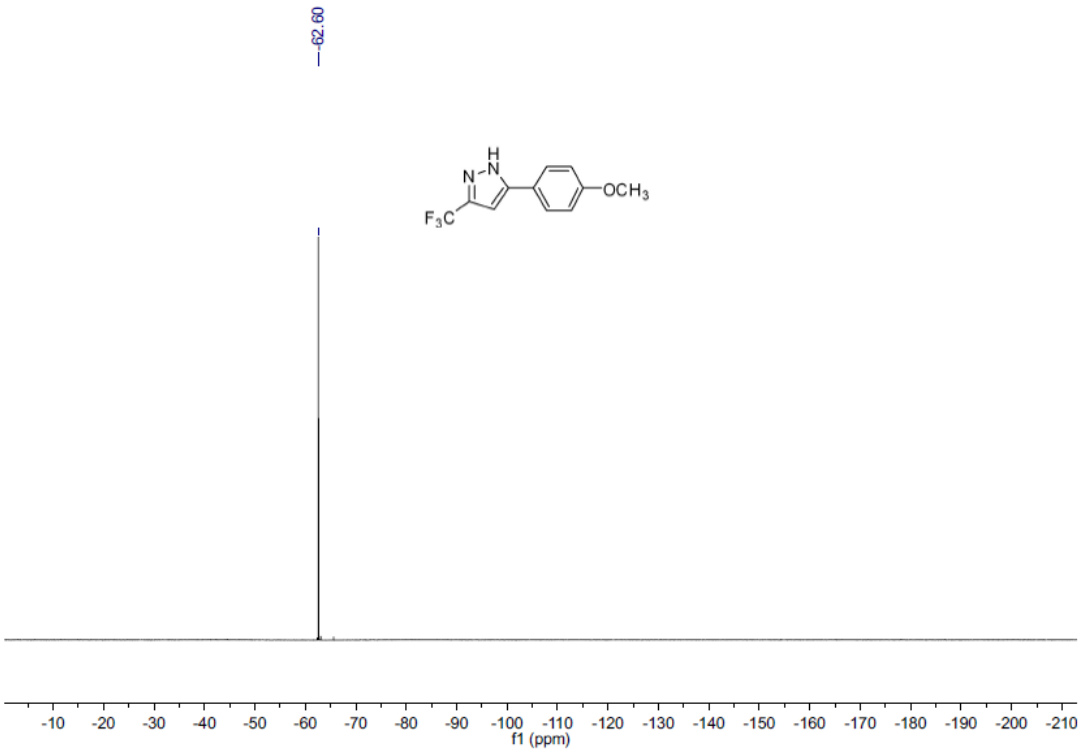
^{1}H NMR copies of compound **4b**:



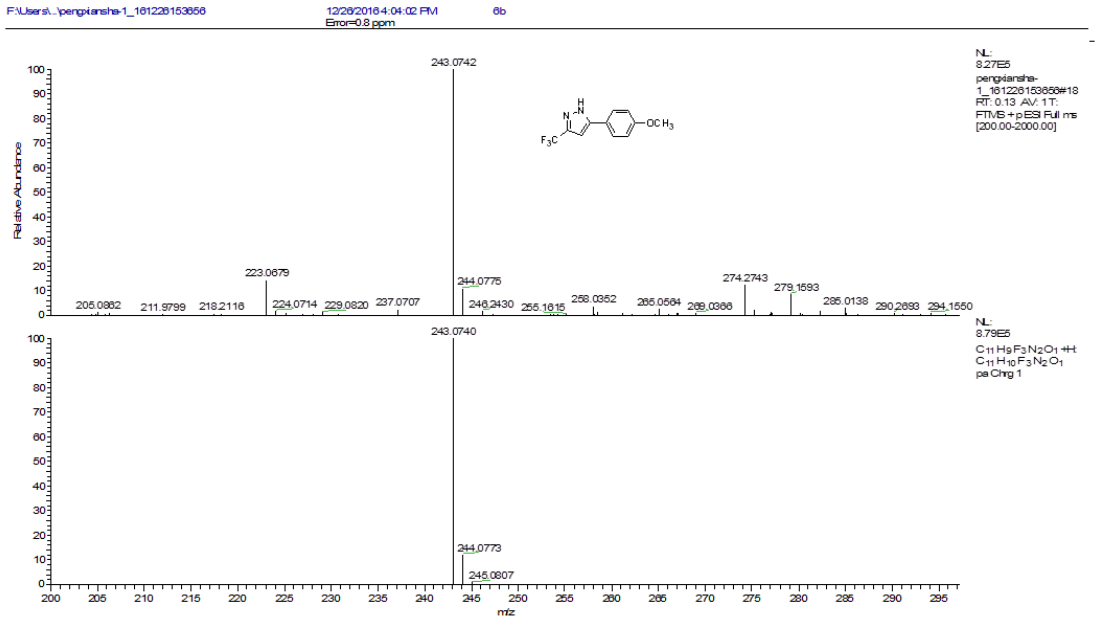
^{13}C NMR copies of compound **4b**:



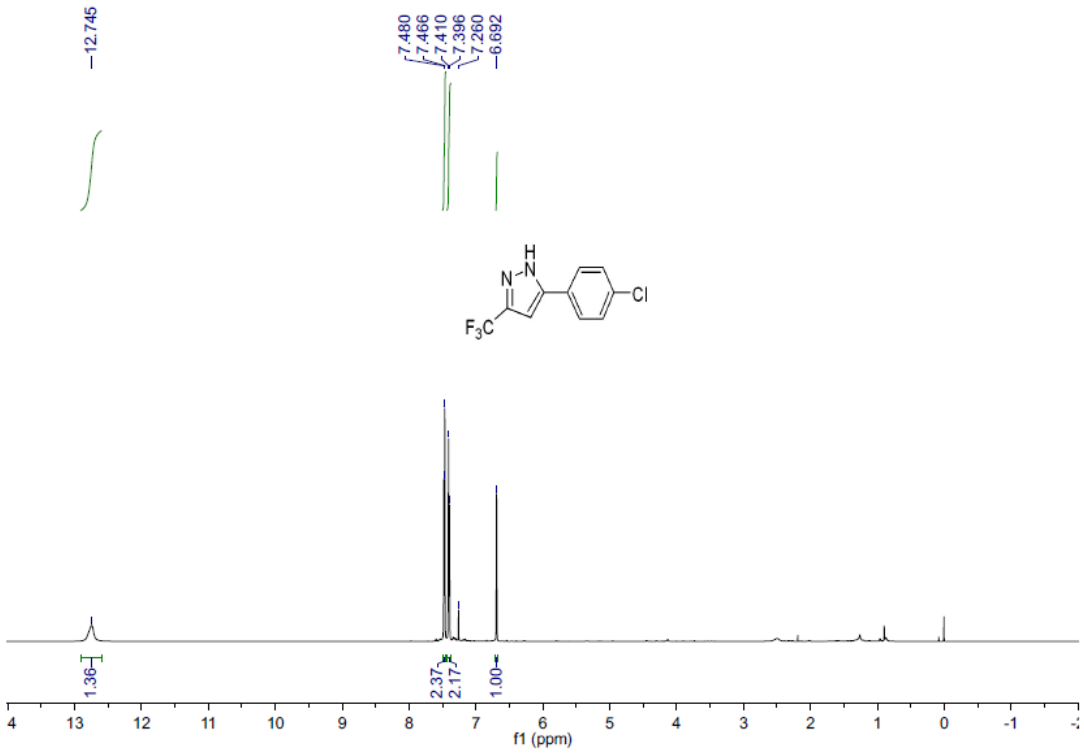
^{19}F NMR copies of compound **4b**:



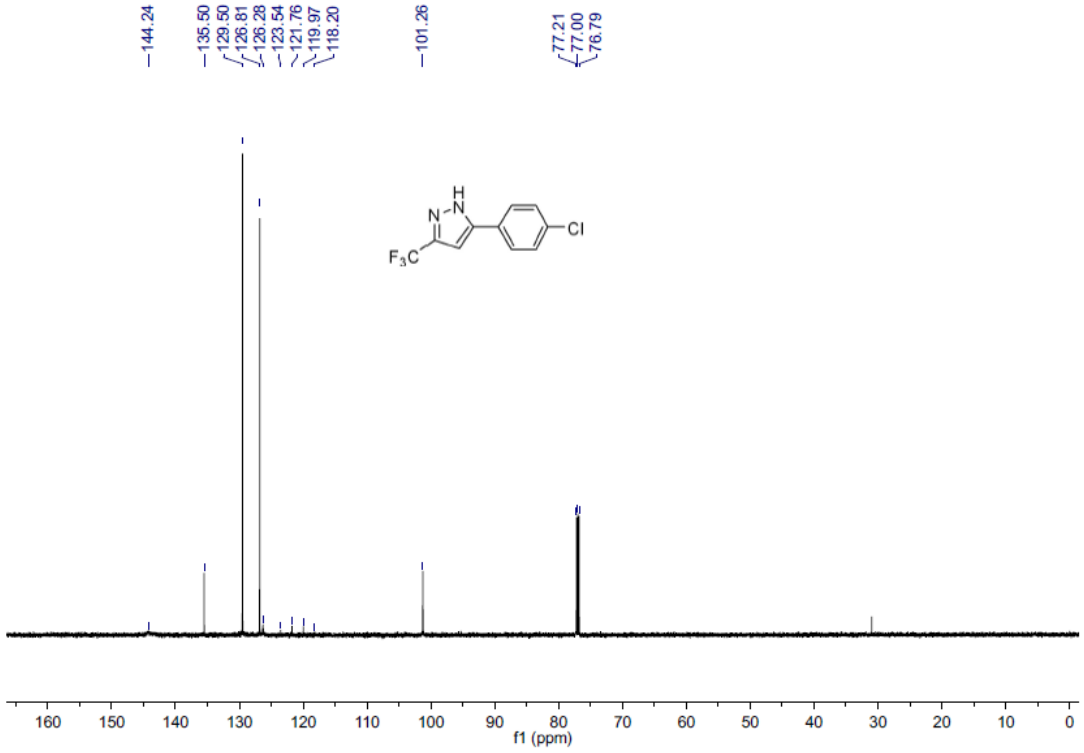
HRMS (ESI) of compound **4b**:



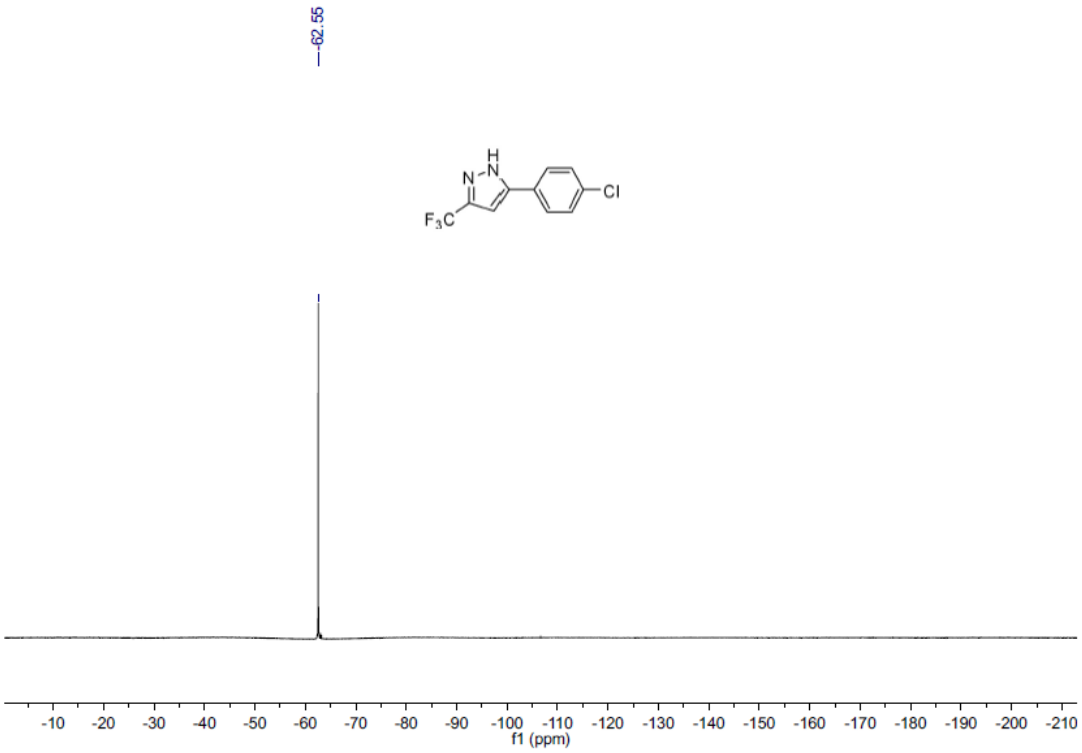
^{1}H NMR copies of compound **4c**:



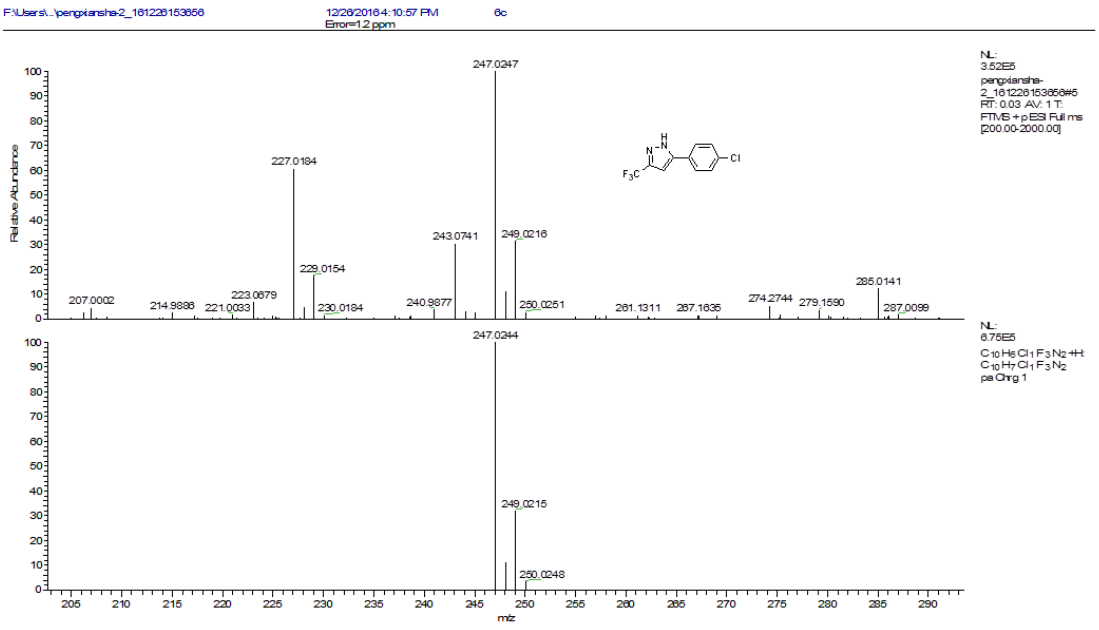
^{13}C NMR copies of compound **4c**:



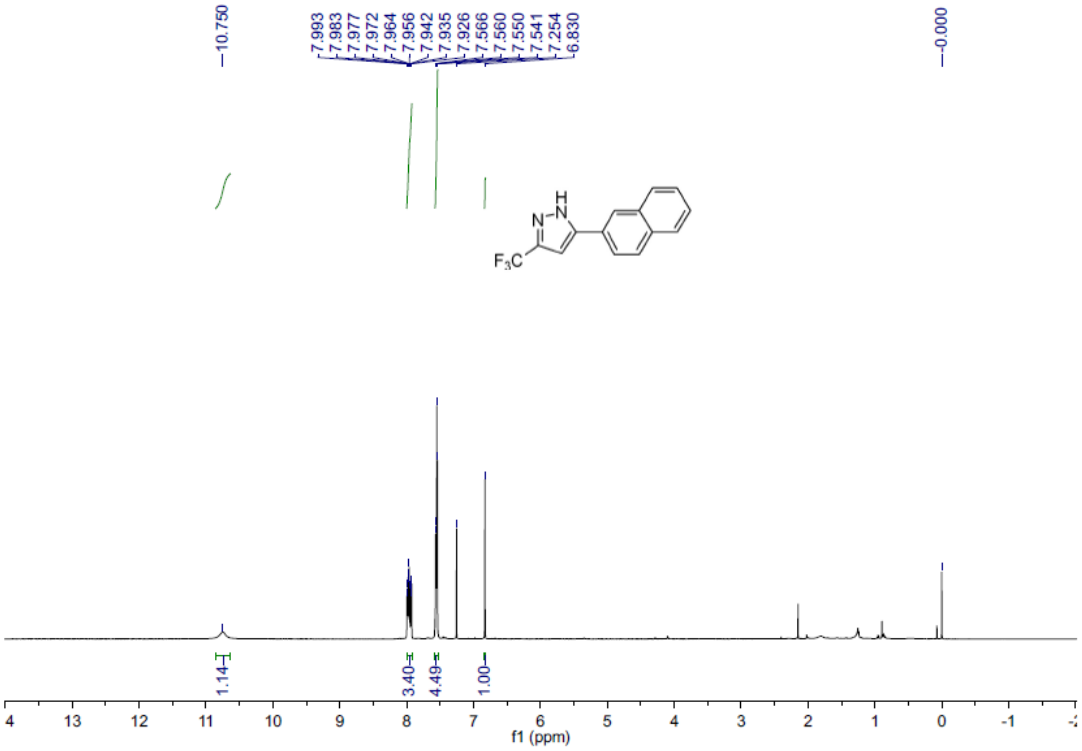
^{19}F NMR copies of compound **4c**:



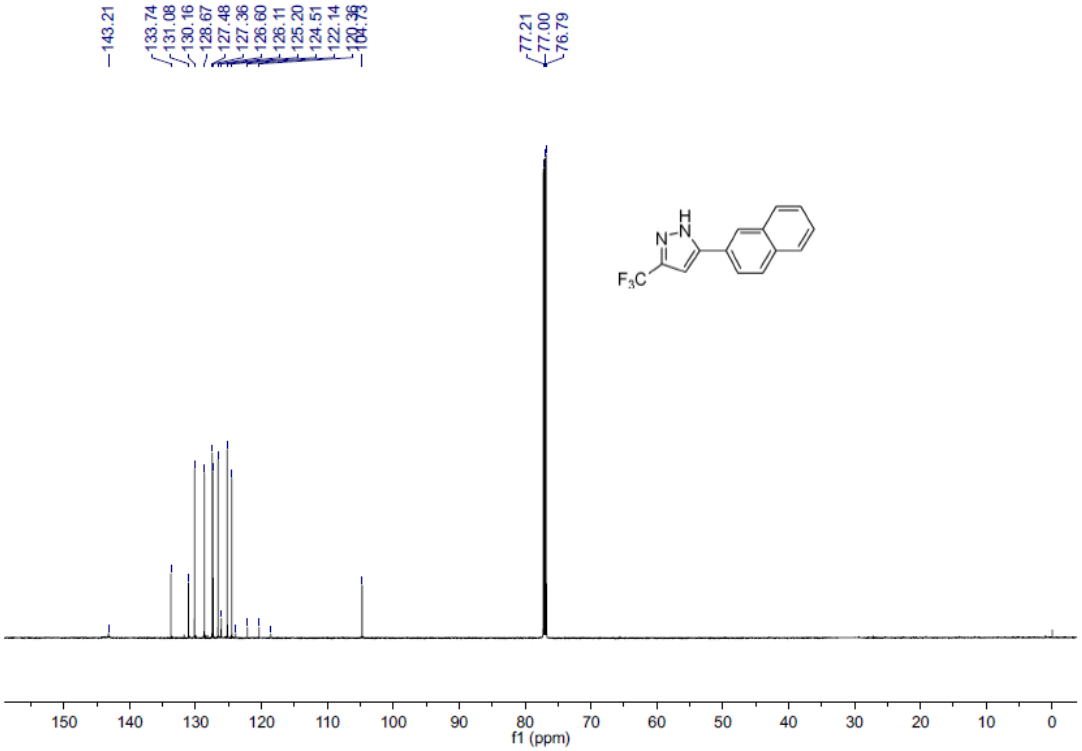
HRMS (ESI) of compound **4c**:



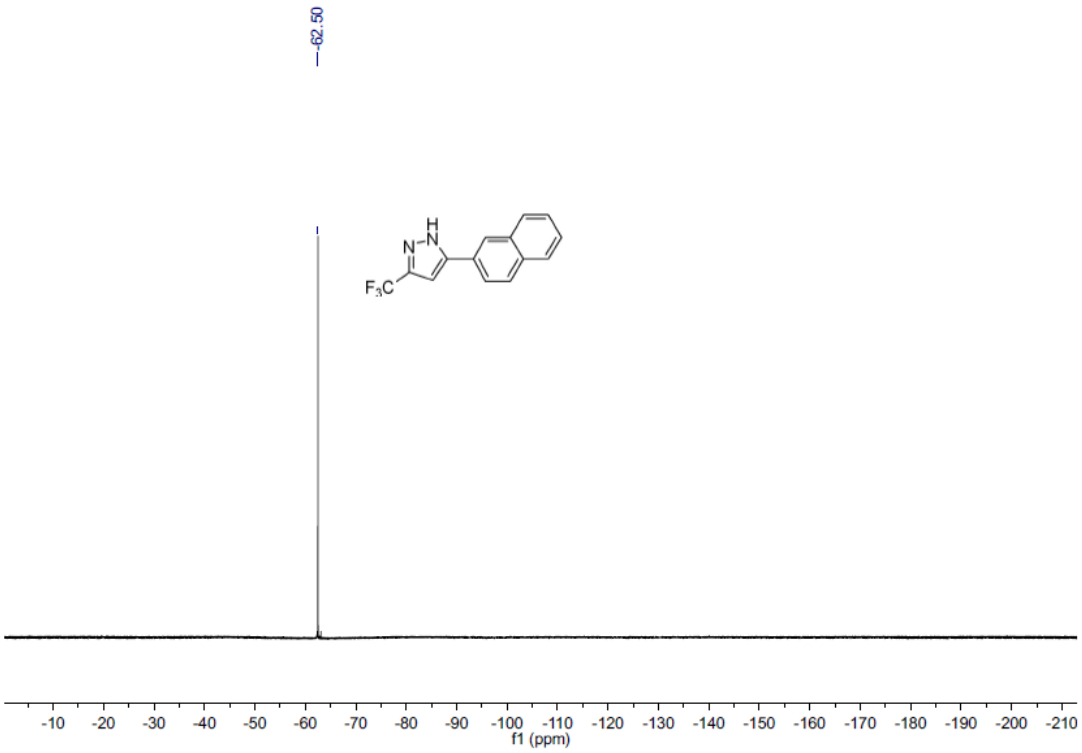
^{1}H NMR copies of compound **4d**:



^{13}C NMR copies of compound **4d**:



^{19}F NMR copies of compound **4d**:



HRMS (ESI) of compound **4d**: