Synthesis and *in vitro* antibacterial evaluation of Mannich-base nitrothiazole derivatives

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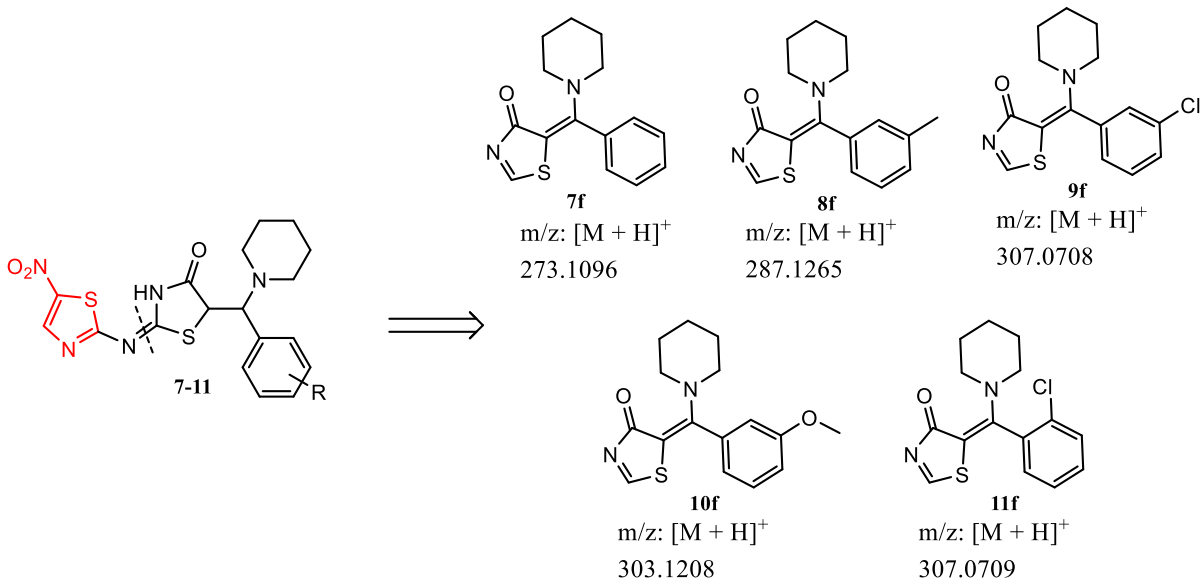


Scheme S1: Structures of fragments formed during ionization.

Compound 7, (E)-2-((5-nitrothiazol-2-yl)imino)-5-(phenyl(piperidin-1-yl)methyl)thiazolidin-4-one

Figure S1, ^{1}H NMR spectrum of compound 7

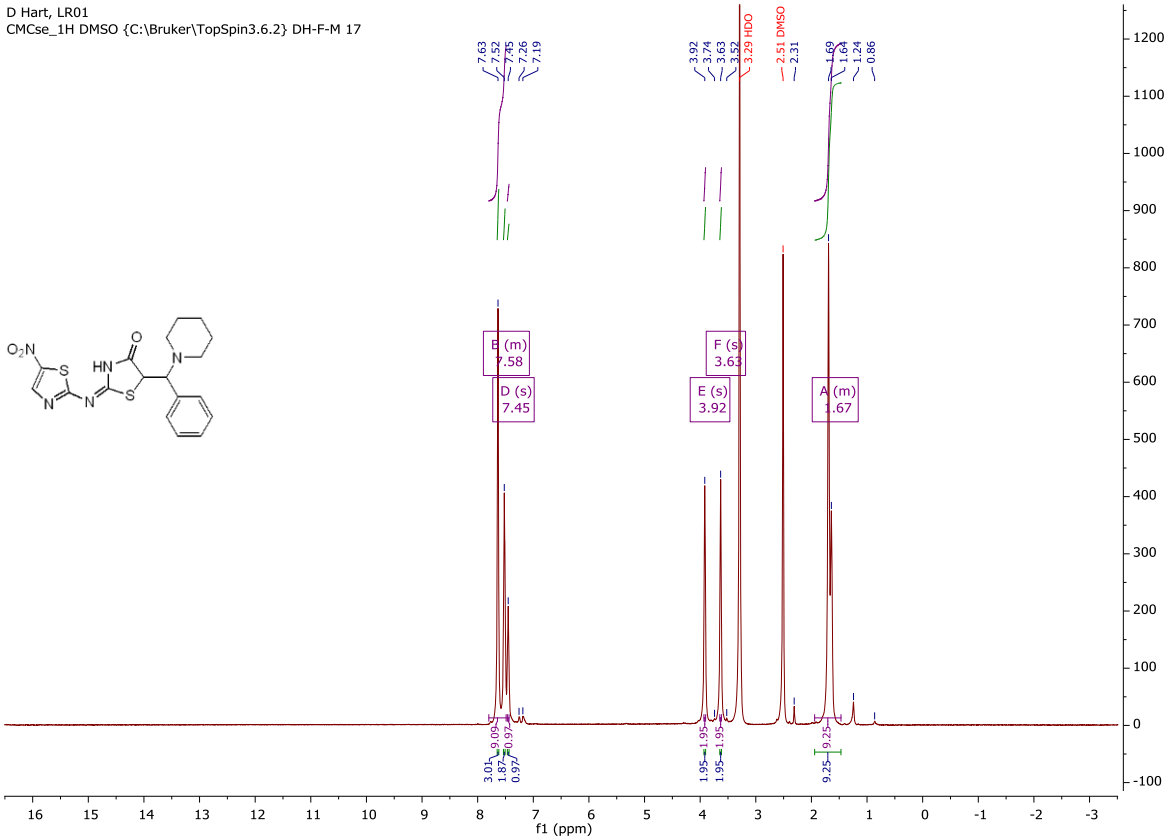


Figure S2, ^{13}C NMR spectrum of Compound 7

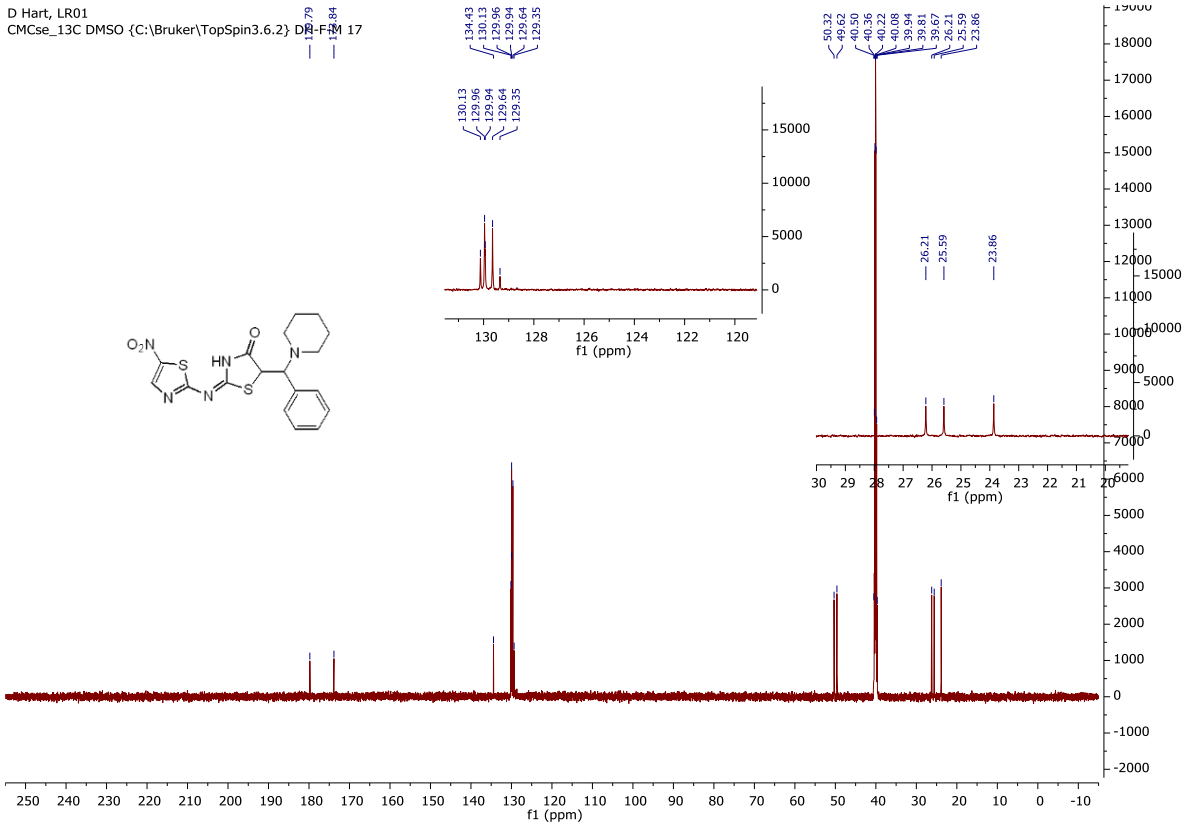
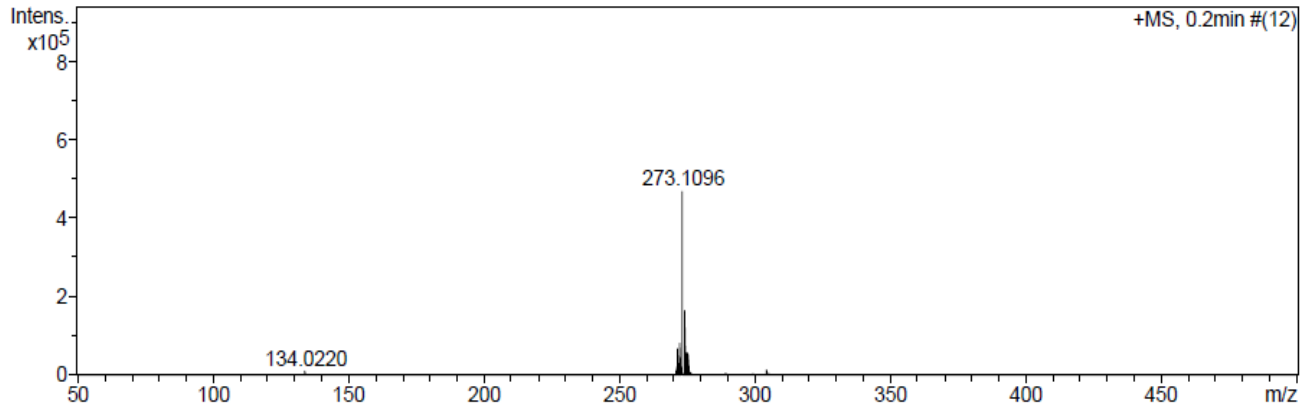


Figure S3, HRMS of compound 7

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
273.1096	1	C 15 H 17 N 2 O S	8.75	273.1056	-3.9	-14.4	92.8	8.5	even	ok
	2	C 12 H 21 N 2 O S 2	100.00	273.1090	-0.6	-2.1	99.9	3.5	even	ok
	3	C 10 H 19 N 5 S 2	33.72	273.1076	-1.9	-7.0	105.3	4.0	odd	ok
	4	C 17 H 13 N 4	4.58	273.1135	3.9	14.4	107.0	13.5	even	ok
	5	C 14 H 15 N 3 O 3	18.97	273.1108	1.2	4.5	124.9	9.0	odd	ok

Compound 8, (E)-2-((5-nitrothiazol-2-yl)imino)-5-(piperidin-1-yl(m-tolyl)methyl)thiazolidin-4-one

Figure S4, ^{1}H NMR spectrum of compound 8

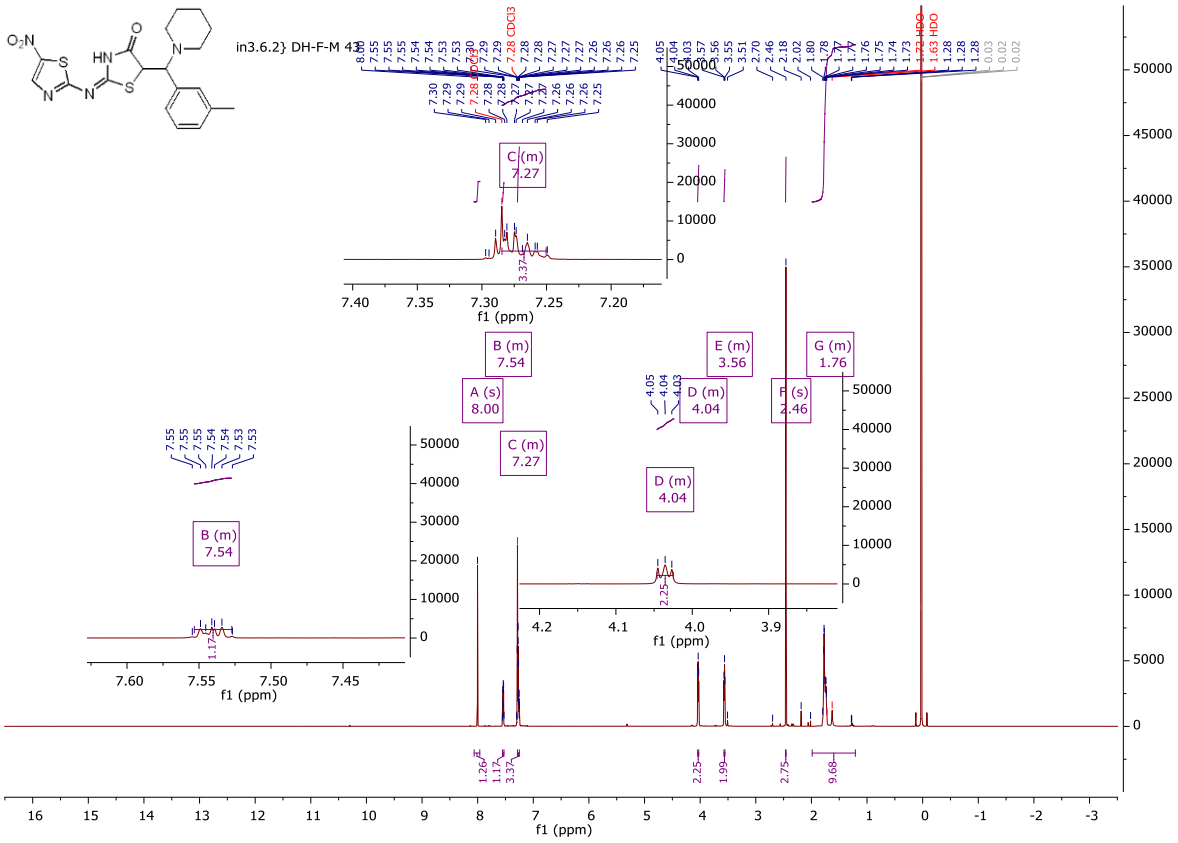


Figure S5, ^{13}C NMR spectrum of compound 8

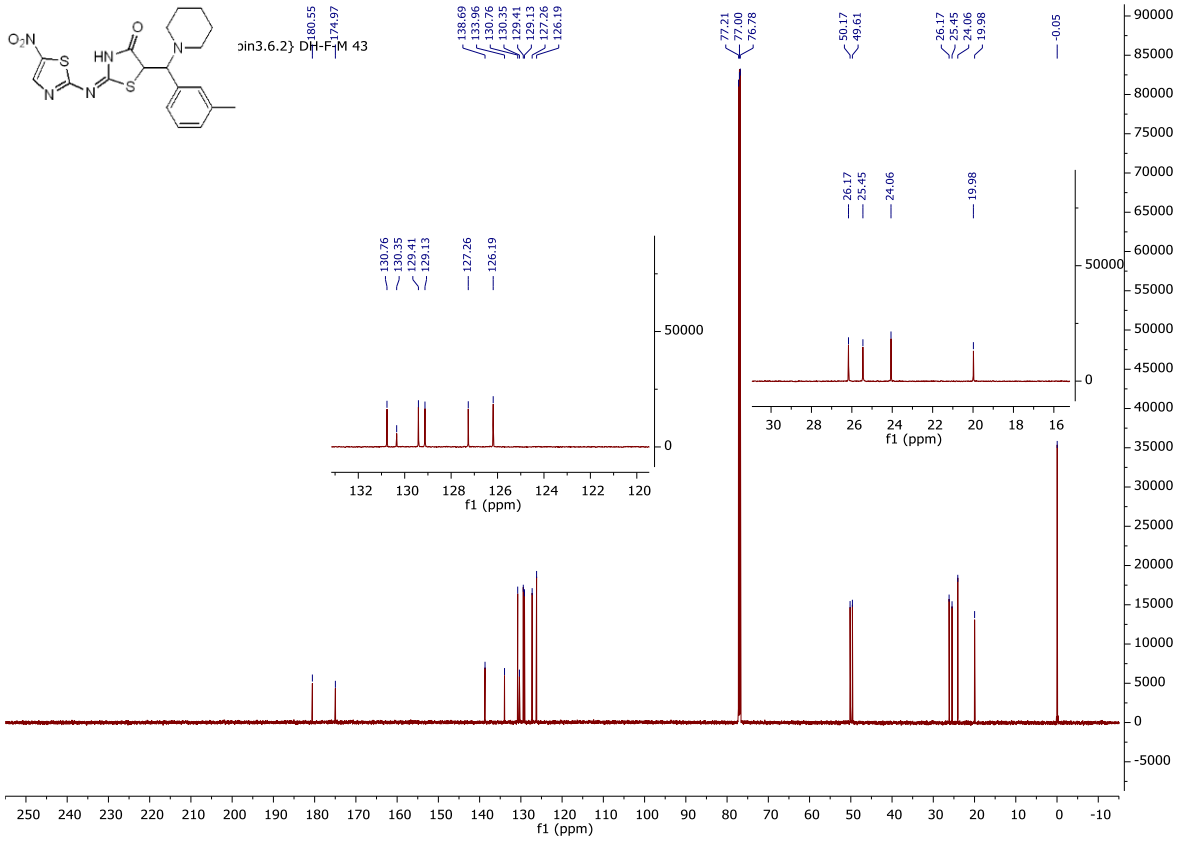
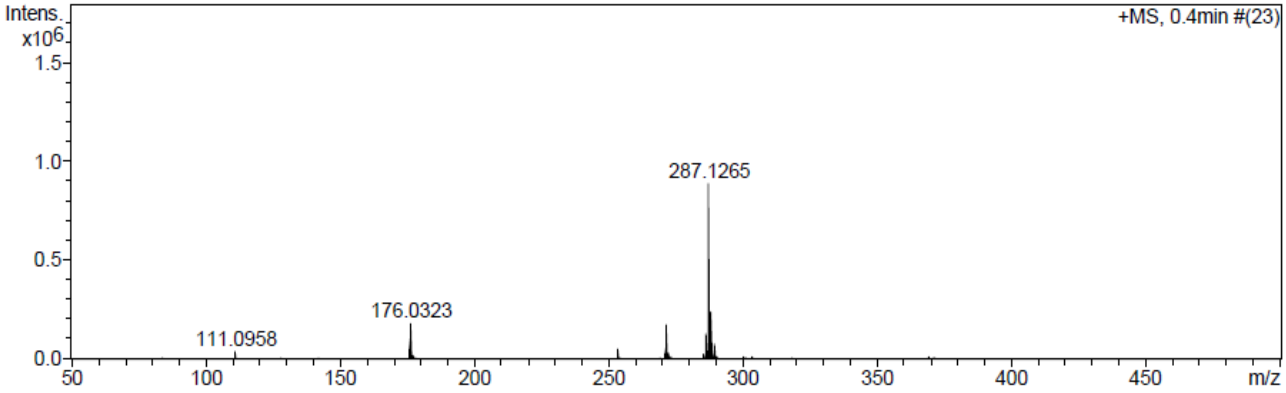


Figure S6, HRMS of compound 8

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
287.1265	1	C 18 H 15 N 4	31.44	287.1291	2.7	9.3	52.4	13.5	even	ok
	2	C 13 H 23 N 2 O S 2	59.56	287.1246	-1.8	-6.3	54.1	3.5	even	ok
	3	C 11 H 21 N 5 S 2	15.80	287.1233	-3.2	-11.0	59.2	4.0	odd	ok
	4	C 12 H 21 N 3 O 3 S	11.52	287.1298	3.4	11.7	62.5	4.0	odd	ok
	5	C 15 H 17 N 3 O 3	100.00	287.1264	-0.0	-0.0	68.5	9.0	odd	ok

Compound 9, (E)-5-((3-chlorophenyl)(piperidin-1-yl)methyl)-2-((5-nitrothiazol-2-yl)imino)thiazolidin-4-one

Figure S7, ^{1}H NMR spectrum of compound 9

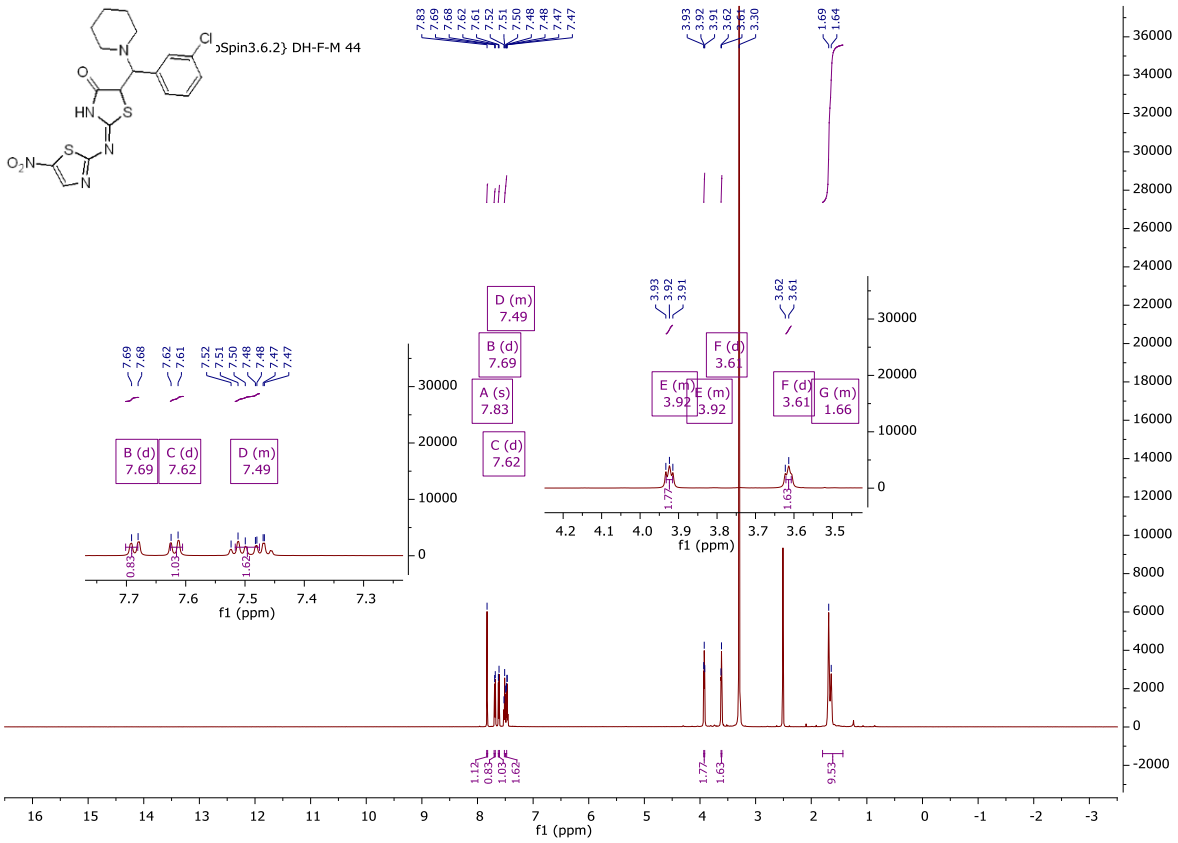


Figure S8, ^{13}C NMR spectrum of compound 9

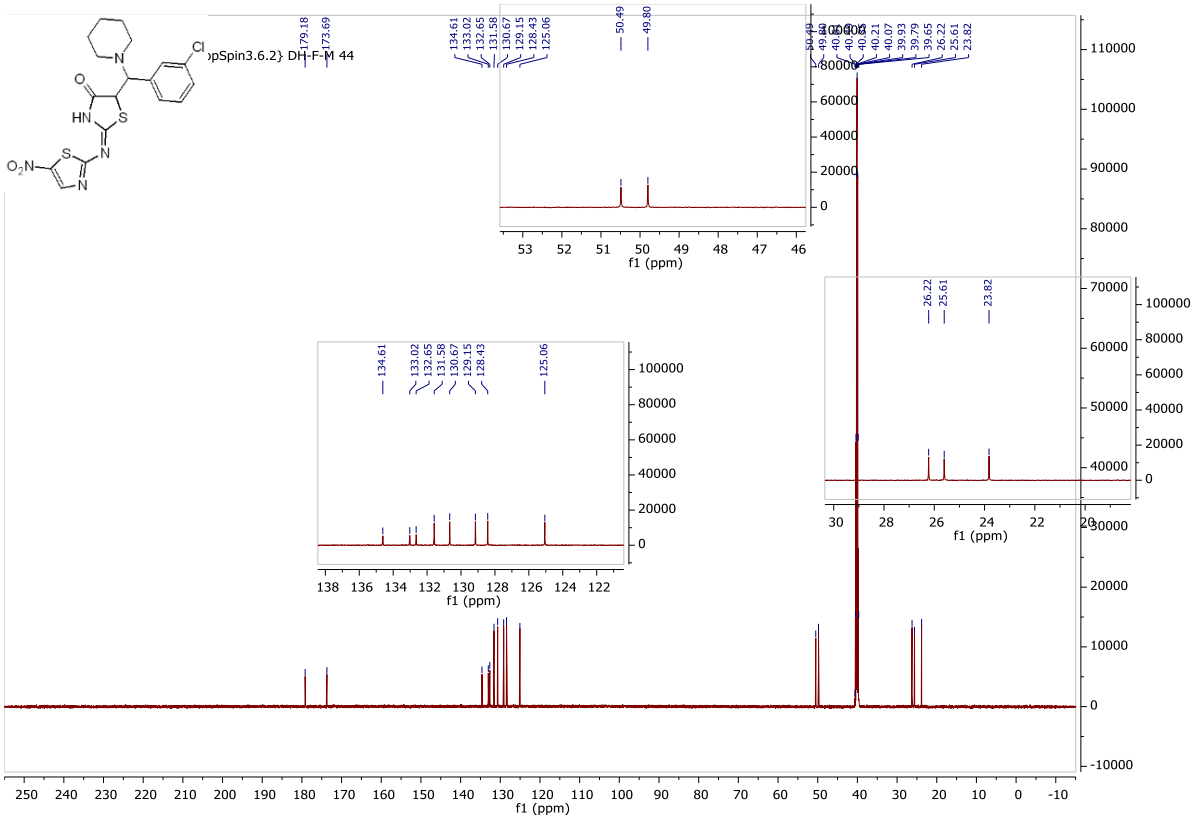
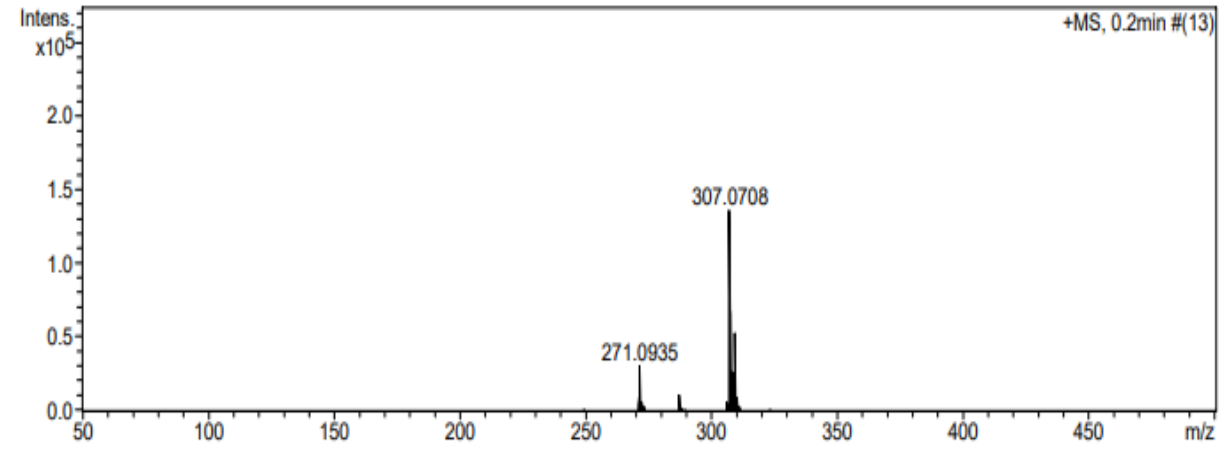


Figure S9, HRMS of compound 9

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
307.0708	1	C 12 H 20 Cl N 2 O S 2	100.00	307.0700	-0.8	-2.5	22.8	3.5	even	ok

Compound 10, (E)-5-((3-methoxyphenyl)(piperidin-1-yl)methyl)-2-((5-nitrothiazol-2-yl)imino)thiazolidin-4-one

Figure S10, ^{1}H NMR spectrum of compound 10

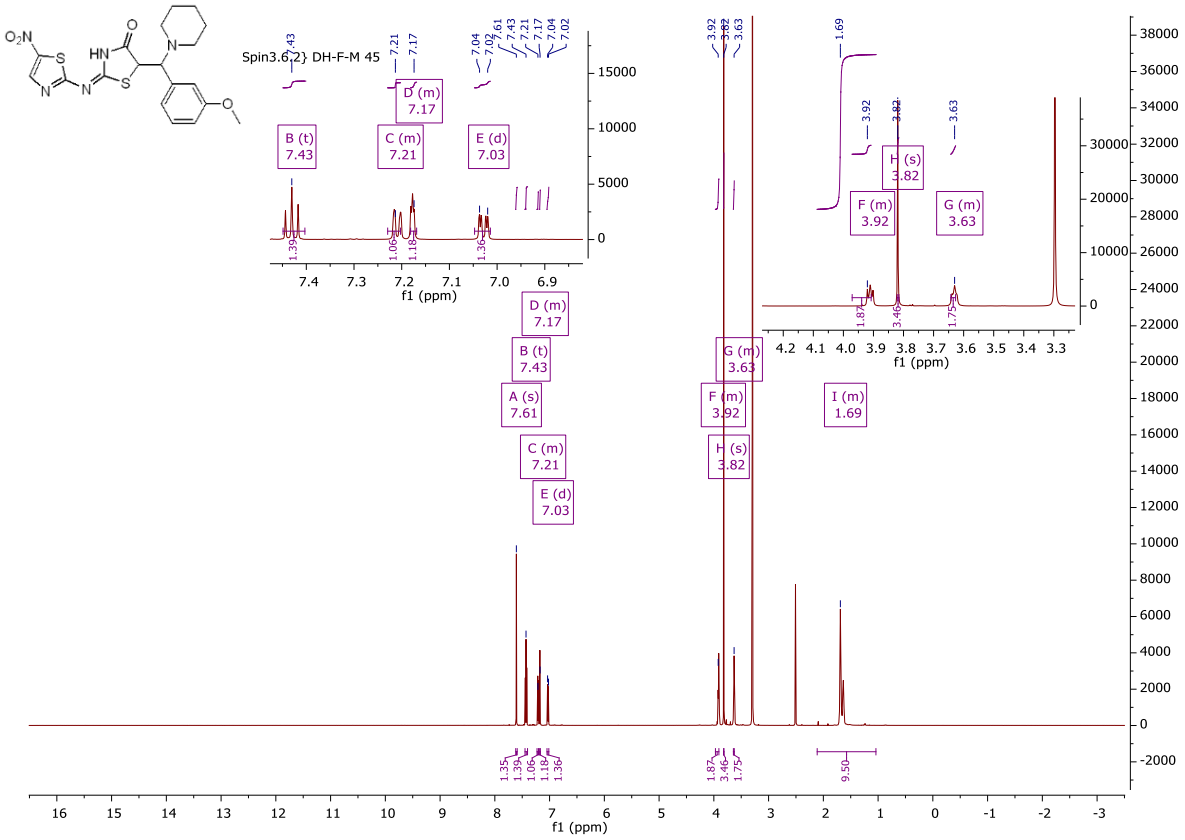


Figure S11, ^{13}C NMR spectrum of compound 10

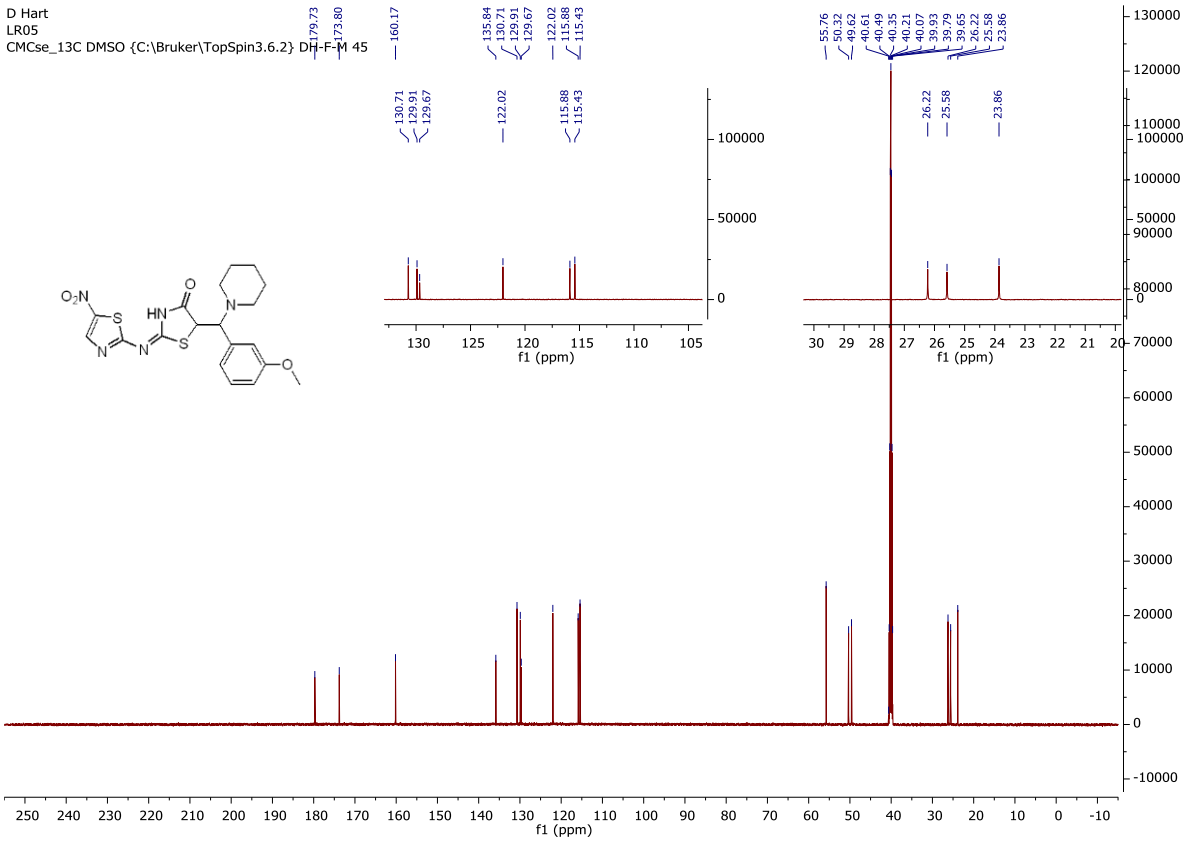
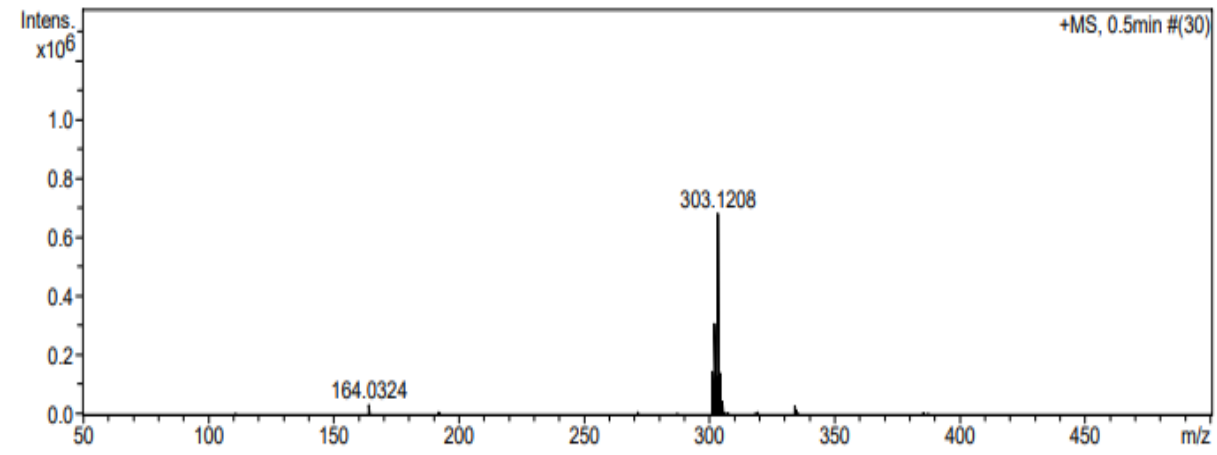


Figure S12, HRMS of compound 10

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z # Formula Score m/z err [mDa] err [ppm] mSigma rdb e⁻ Conf N-Rule

Compound 11, (E)-5-((2-chlorophenyl)(piperidin-1-yl)methyl)-2-((5-nitrothiazol-2-yl)imino)thiazolidin-4-one

Figure S13, ^{1}H NMR spectrum of compound 11

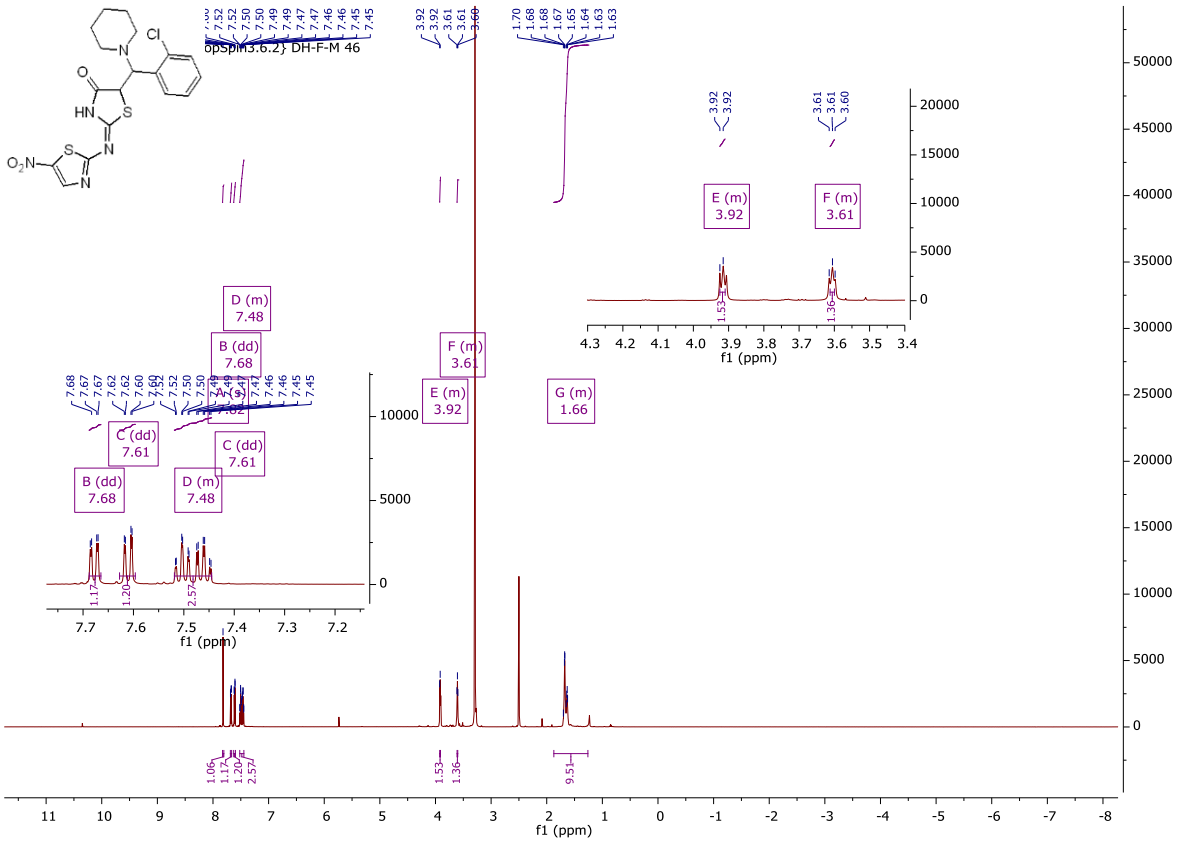


Figure S14, ^{13}C NMR spectrum of compound 11

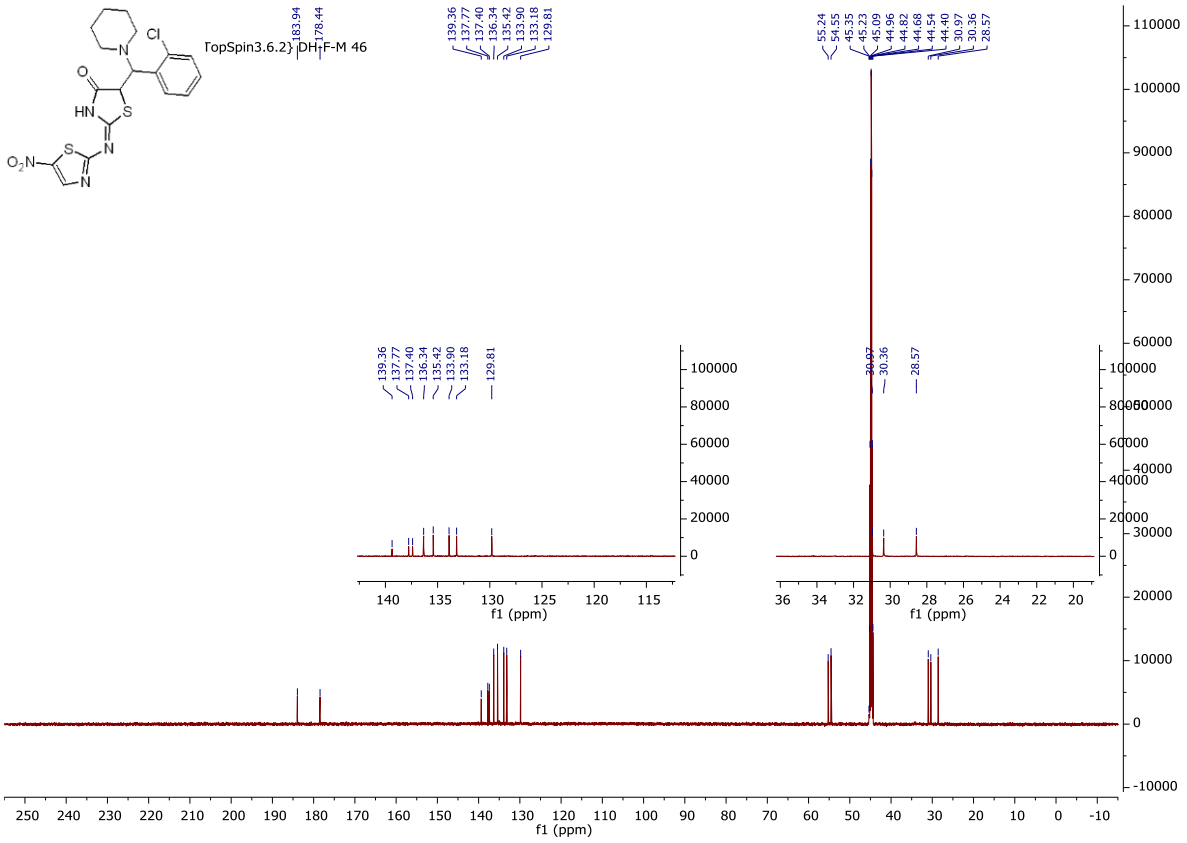


Figure S15, HRMS of compound 11

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste