Supplementary Information

for

A Mild One-Pot Synthesis to 2-Iminothiazolines from Thioureas and 1-Bromo-1-nitroalkenes

Yuan Xu,[a,b] Xin Ge,[b] Yuhan Zhang,[b] Hongbin Zhang,[a] and Xue-Wei Liu[b,*]

[a] Key Laboratory of Medicinal Chemistry for Natural Resource, Ministry of Education and Yunnan Province, School of Chemical Science and Technology, Yunnan University, Kunming 650091, China;
[b] Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371.

Email: xuewei@ntu.edu.sg

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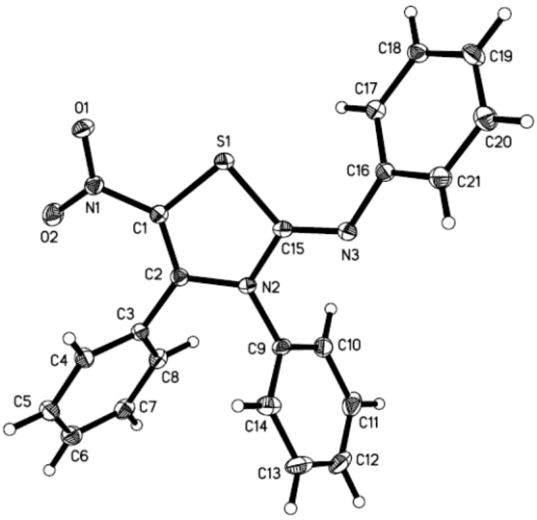
1. X-ray data of compound 3a



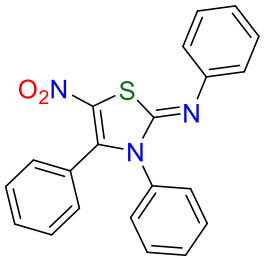


Table S1. Crystal data and structure refinement for compound **3a**.

Identification code	**3a**	
Empirical formula	C21 H15 N3 O2 S	
Formula weight	373.42	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.5389(5) Å b = 9.3143(2) Å c = 18.8825(4) Å	a= 90°. b= 103.7740(10)°. g = 90°.
Volume	3508.44(14) Å ^{3}	
Z	8	
Density (calculated)	1.414 Mg/m ^{3}	
Absorption coefficient	0.207 mm^{-1}	
F(000)	1552	
Crystal size	0.40 x 0.40 x 0.20 mm^3	
Theta range for data collection	2.04 to 31.03°.	

Index ranges	-29<=h<=29, -7<=k<=13, -26<=l<=27
Reflections collected	26512
Independent reflections	5604 [R(int) = 0.0259]
Completeness to theta = 31.03°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9598 and 0.9219
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5604 / 0 / 244
Goodness-of-fit on F^2	1.169
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.1008
R indices (all data)	R1 = 0.0508, wR2 = 0.1265
Largest diff. peak and hole	0.690 and -0.562 e.Å $^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å $^2\times 10^3$) for liu76s. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1747(1)	7370(1)	1985(1)	15(1)
C(2)	1595(1)	7296(1)	2650(1)	14(1)
C(3)	1712(1)	6112(1)	3185(1)	14(1)
C(4)	1452(1)	4755(1)	2973(1)	16(1)
C(5)	1534(1)	3651(1)	3480(1)	19(1)
C(6)	1867(1)	3904(2)	4201(1)	20(1)
C(7)	2130(1)	5251(2)	4412(1)	19(1)
C(8)	2055(1)	6361(1)	3907(1)	16(1)
C(9)	1015(1)	8721(1)	3426(1)	15(1)
C(10)	1314(1)	9738(2)	3934(1)	18(1)
C(11)	1092(1)	9884(2)	4571(1)	25(1)
C(12)	586(1)	9003(2)	4696(1)	27(1)
C(13)	285(1)	8005(2)	4176(1)	26(1)
C(14)	496(1)	7859(2)	3532(1)	20(1)
C(15)	1176(1)	9581(1)	2244(1)	13(1)
C(16)	811(1)	11833(1)	1777(1)	15(1)
C(17)	1354(1)	12329(1)	1520(1)	16(1)
C(18)	1271(1)	13473(1)	1034(1)	18(1)
C(19)	655(1)	14146(2)	811(1)	21(1)
C(20)	114(1)	13662(2)	1072(1)	23(1)
C(21)	190(1)	12512(2)	1554(1)	19(1)
N(1)	2113(1)	6370(1)	1672(1)	16(1)
N(2)	1268(1)	8518(1)	2785(1)	13(1)
N(3)	876(1)	10746(1)	2309(1)	15(1)
O(1)	2108(1)	6562(1)	1018(1)	20(1)
O(2)	2416(1)	5379(1)	2040(1)	20(1)
S(1)	1503(1)	8959(1)	1511(1)	15(1)

Table S3. Bond lengths [Å] and angles [°] for liu76s.

C(1)-C(2)	1.3656(16)
C(1)-N(1)	1.4125(16)
C(1)-S(1)	1.7401(13)
C(2)-N(2)	1.3756(16)
C(2)-C(3)	1.4761(17)
C(3)-C(4)	1.3927(17)
C(3)-C(8)	1.3978(17)
C(4)-C(5)	1.3884(18)
C(4)-H(4)	0.9500
C(5)-C(6)	1.391(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.387(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.3892(18)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(10)	1.3829(18)
C(9)-C(14)	1.3865(18)
C(9)-N(2)	1.4402(15)
C(10)-C(11)	1.3900(18)
C(10)-H(10)	0.9500
C(11)-C(12)	1.386(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.386(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.3922(19)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-N(3)	1.2687(16)
C(15)-N(2)	1.4030(15)
C(15)-S(1)	1.7714(12)
C(16)-C(21)	1.3968(18)
C(16)-C(17)	1.3973(18)
C(16)-N(3)	1.4095(16)
C(17)-C(18)	1.3902(18)
C(17)-H(17)	0.9500
C(18)-C(19)	1.385(2)
C(18)-H(18)	0.9500

C(19)-C(20)	1.392(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.3907(19)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
N(1)-O(2)	1.2307(15)
N(1)-O(1)	1.2454(14)

C(2)-C(1)-N(1)	127.72(11)
C(2)-C(1)-S(1)	114.51(9)
N(1)-C(1)-S(1)	117.60(9)
C(1)-C(2)-N(2)	110.89(11)
C(1)-C(2)-C(3)	129.18(11)
N(2)-C(2)-C(3)	119.89(10)
C(4)-C(3)-C(8)	120.06(12)
C(4)-C(3)-C(2)	119.51(11)
C(8)-C(3)-C(2)	120.37(11)
C(5)-C(4)-C(3)	119.92(12)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	120.02(13)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(7)-C(6)-C(5)	120.09(12)
C(7)-C(6)-H(6)	120.0
C(5)-C(6)-H(6)	120.0
C(6)-C(7)-C(8)	120.31(12)
C(6)-C(7)-H(7)	119.8
C(8)-C(7)-H(7)	119.8
C(7)-C(8)-C(3)	119.58(12)
C(7)-C(8)-H(8)	120.2
C(3)-C(8)-H(8)	120.2
C(10)-C(9)-C(14)	121.75(12)
C(10)-C(9)-N(2)	118.95(11)
C(14)-C(9)-N(2)	119.26(12)
C(9)-C(10)-C(11)	118.92(13)
C(9)-C(10)-H(10)	120.5
C(11)-C(10)-H(10)	120.5
C(12)-C(11)-C(10)	120.18(14)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(13)-C(12)-C(11)	120.19(13)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	120.29(14)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(9)-C(14)-C(13)	118.64(14)

C(9)-C(14)-H(14)	120.7
C(13)-C(14)-H(14)	120.7
N(3)-C(15)-N(2)	121.13(11)
N(3)-C(15)-S(1)	129.69(10)
N(2)-C(15)-S(1)	109.13(9)
C(21)-C(16)-C(17)	119.58(12)
C(21)-C(16)-N(3)	117.70(11)
C(17)-C(16)-N(3)	122.48(11)
C(18)-C(17)-C(16)	120.02(12)
C(18)-C(17)-H(17)	120.0
C(16)-C(17)-H(17)	120.0
C(19)-C(18)-C(17)	120.46(12)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	119.63(13)
C(18)-C(19)-H(19)	120.2
C(20)-C(19)-H(19)	120.2
C(21)-C(20)-C(19)	120.49(13)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(20)-C(21)-C(16)	119.82(13)
C(20)-C(21)-H(21)	120.1
C(16)-C(21)-H(21)	120.1
O(2)-N(1)-O(1)	123.45(11)
O(2)-N(1)-C(1)	120.47(10)
O(1)-N(1)-C(1)	116.07(11)
C(2)-N(2)-C(15)	115.85(10)
C(2)-N(2)-C(9)	123.66(10)
C(15)-N(2)-C(9)	120.48(10)
C(15)-N(3)-C(16)	120.72(11)
C(1)-S(1)-C(15)	89.60(6)

Symmetry transformations used to generate equivalent atoms.

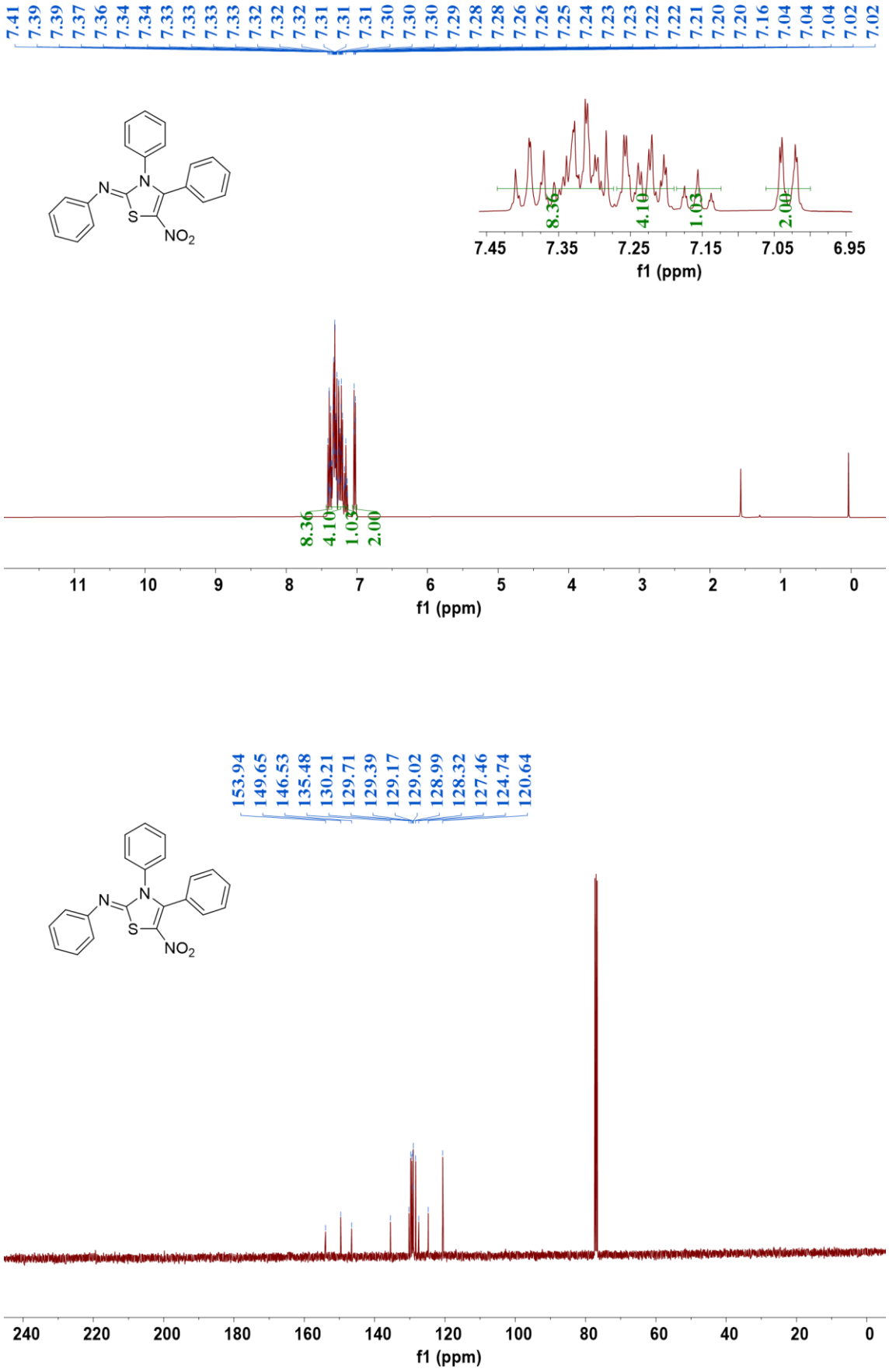
Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for liu76s. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

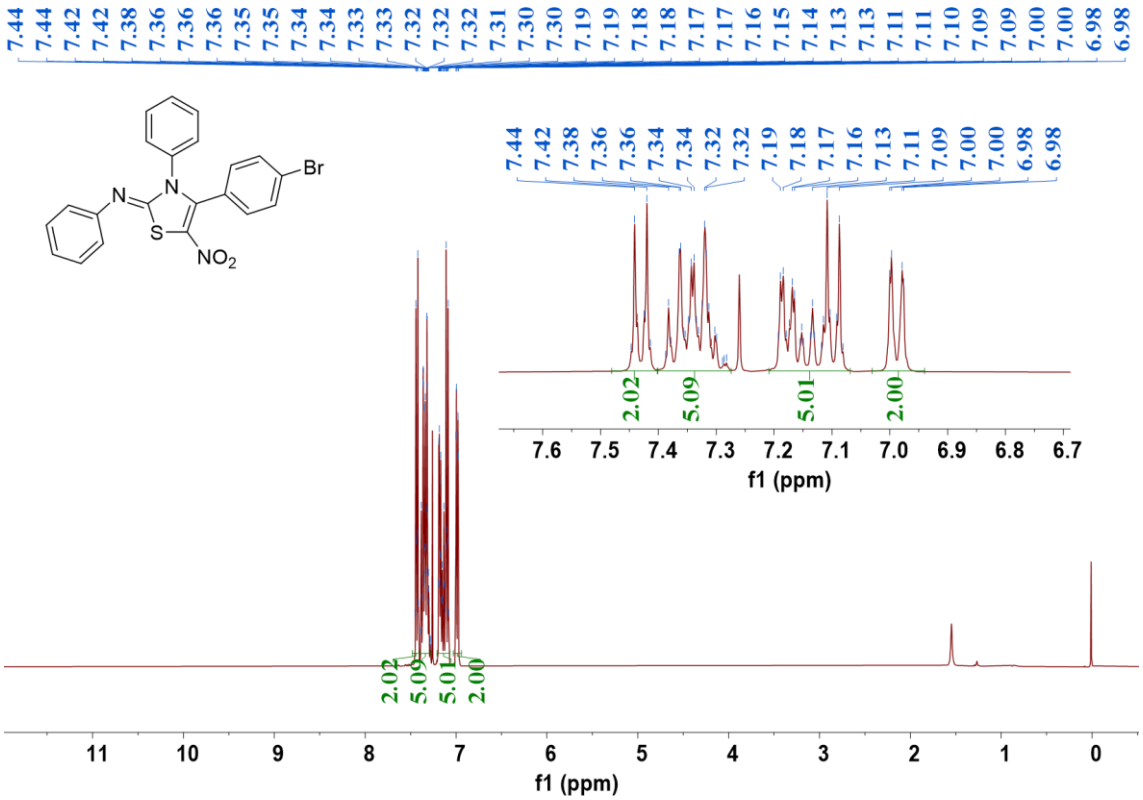
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	13(1)	14(1)	0(1)	5(1)	0(1)
C(2)	14(1)	13(1)	14(1)	0(1)	3(1)	-1(1)
C(3)	14(1)	14(1)	14(1)	1(1)	5(1)	1(1)
C(4)	17(1)	14(1)	16(1)	0(1)	4(1)	0(1)
C(5)	20(1)	15(1)	23(1)	2(1)	7(1)	0(1)
C(6)	23(1)	21(1)	20(1)	7(1)	8(1)	6(1)
C(7)	20(1)	24(1)	14(1)	2(1)	4(1)	6(1)
C(8)	16(1)	18(1)	15(1)	-2(1)	4(1)	2(1)
C(9)	17(1)	17(1)	12(1)	4(1)	6(1)	4(1)
C(10)	24(1)	17(1)	15(1)	1(1)	6(1)	4(1)
C(11)	36(1)	24(1)	16(1)	0(1)	8(1)	11(1)
C(12)	31(1)	35(1)	19(1)	10(1)	14(1)	19(1)
C(13)	19(1)	36(1)	25(1)	14(1)	12(1)	8(1)
C(14)	17(1)	25(1)	19(1)	6(1)	5(1)	1(1)
C(15)	14(1)	15(1)	11(1)	1(1)	4(1)	-2(1)
C(16)	18(1)	13(1)	12(1)	0(1)	4(1)	0(1)
C(17)	18(1)	15(1)	16(1)	1(1)	5(1)	0(1)
C(18)	23(1)	14(1)	17(1)	-1(1)	8(1)	-3(1)
C(19)	29(1)	17(1)	18(1)	5(1)	6(1)	2(1)
C(20)	23(1)	24(1)	23(1)	7(1)	5(1)	6(1)
C(21)	18(1)	20(1)	20(1)	3(1)	6(1)	2(1)
N(1)	15(1)	16(1)	17(1)	-3(1)	6(1)	-2(1)
N(2)	17(1)	13(1)	11(1)	1(1)	6(1)	1(1)
N(3)	16(1)	15(1)	15(1)	2(1)	5(1)	1(1)
O(1)	29(1)	20(1)	15(1)	-2(1)	11(1)	-3(1)
O(2)	19(1)	21(1)	22(1)	1(1)	6(1)	6(1)
S(1)	20(1)	15(1)	12(1)	1(1)	6(1)	0(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for liu76s.

	x	y	z	U(eq)
H(4)	1220	4585	2481	19
H(5)	1361	2722	3335	23
H(6)	1914	3153	4550	25
H(7)	2363	5416	4903	23
H(8)	2236	7283	4052	19
H(10)	1666	10326	3850	22
H(11)	1286	10589	4921	30
H(12)	446	9085	5138	32
H(13)	-67	7417	4261	31
H(14)	289	7183	3172	24
H(17)	1781	11886	1678	19
H(18)	1640	13795	853	21
H(19)	601	14932	482	26
H(20)	-309	14122	920	28
H(21)	-181	12189	1731	23

2. ^{1}H and ^{13}C NMR of compounds 3a-3n

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S
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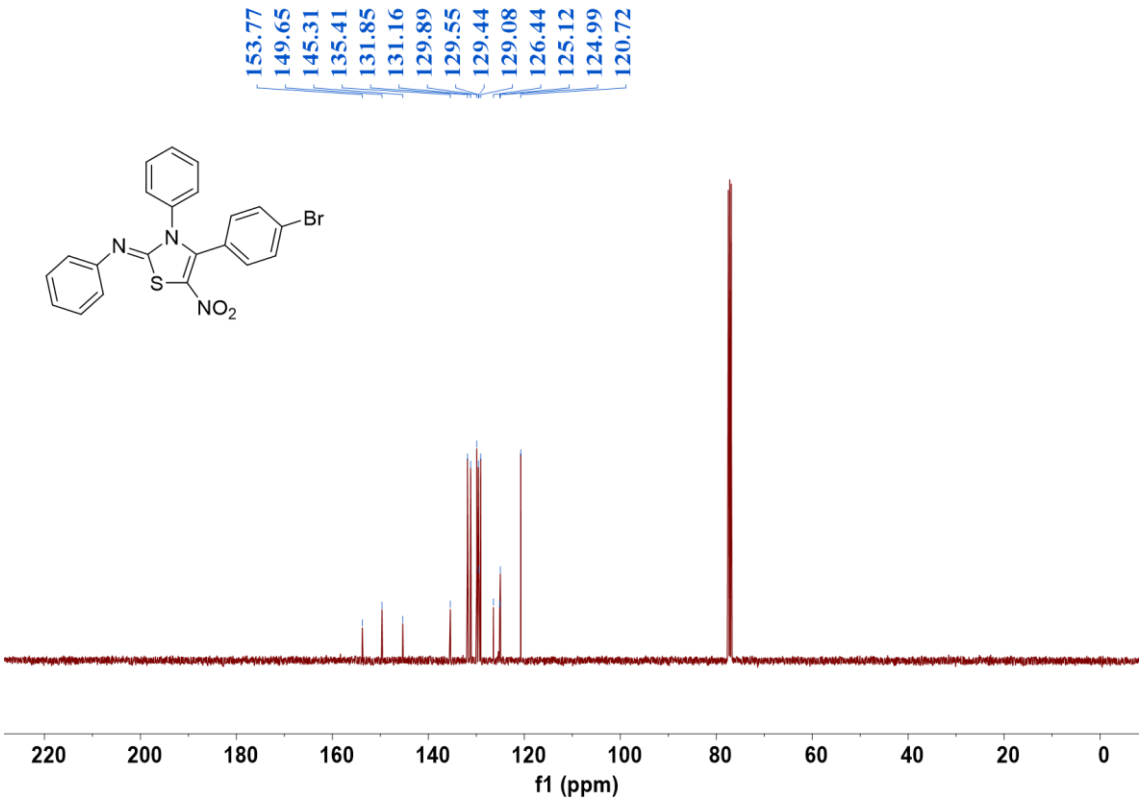
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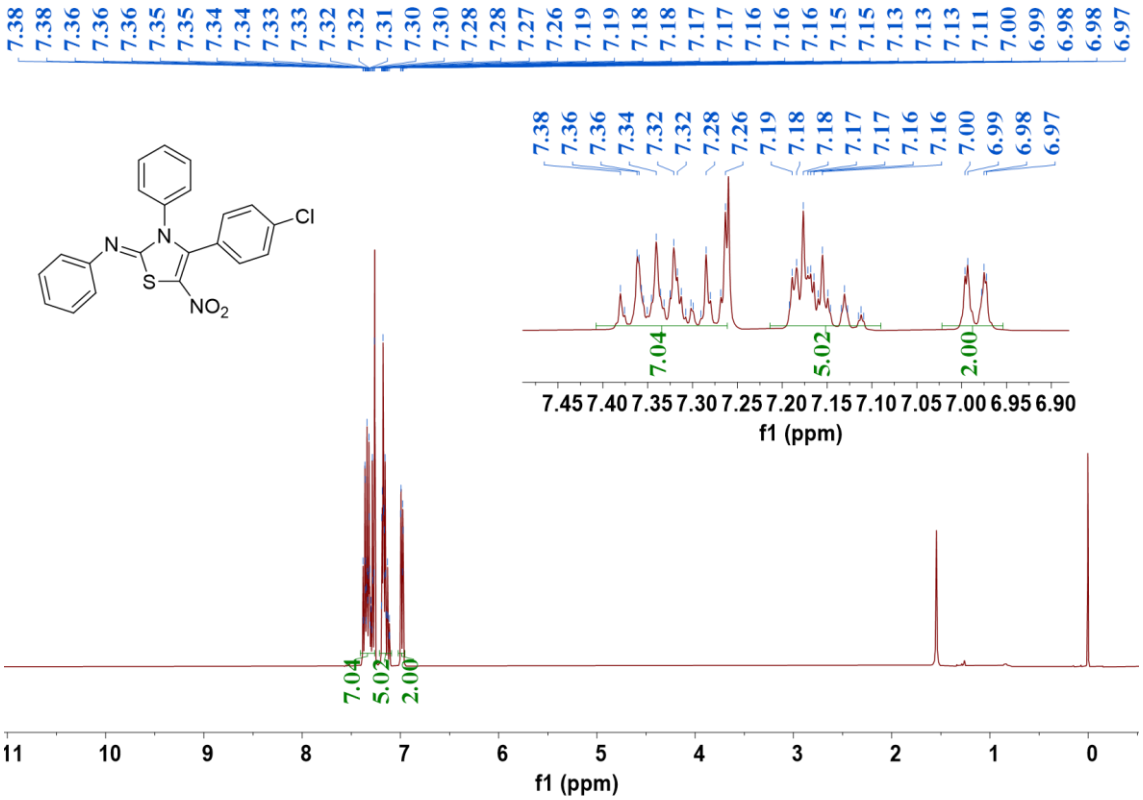
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Cl
N
S
NO2
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7.04
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2.00
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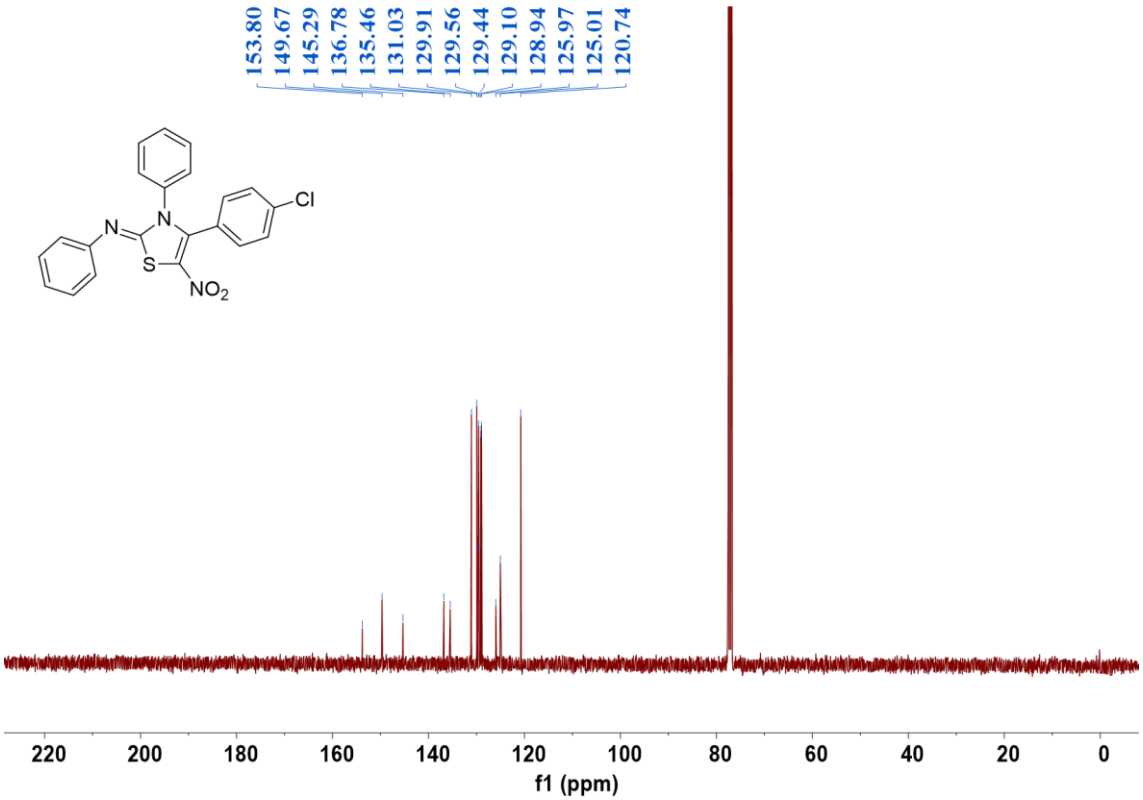
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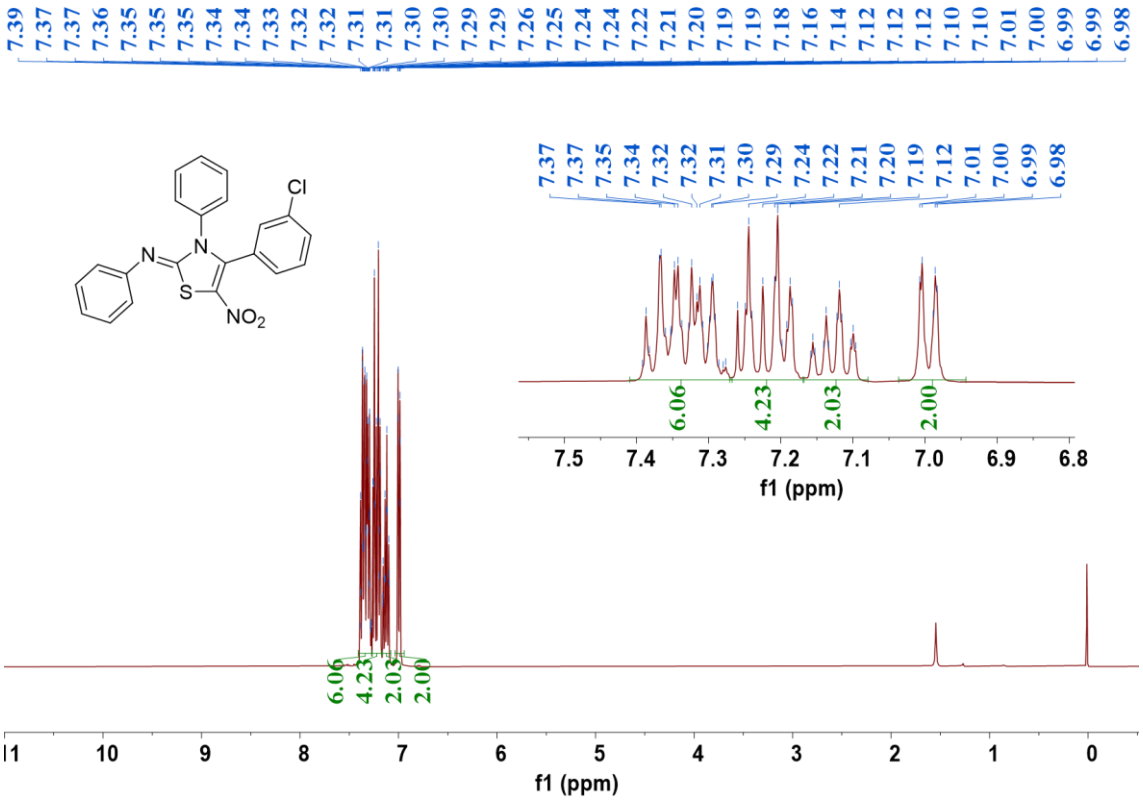
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Cl
N
S
NO2
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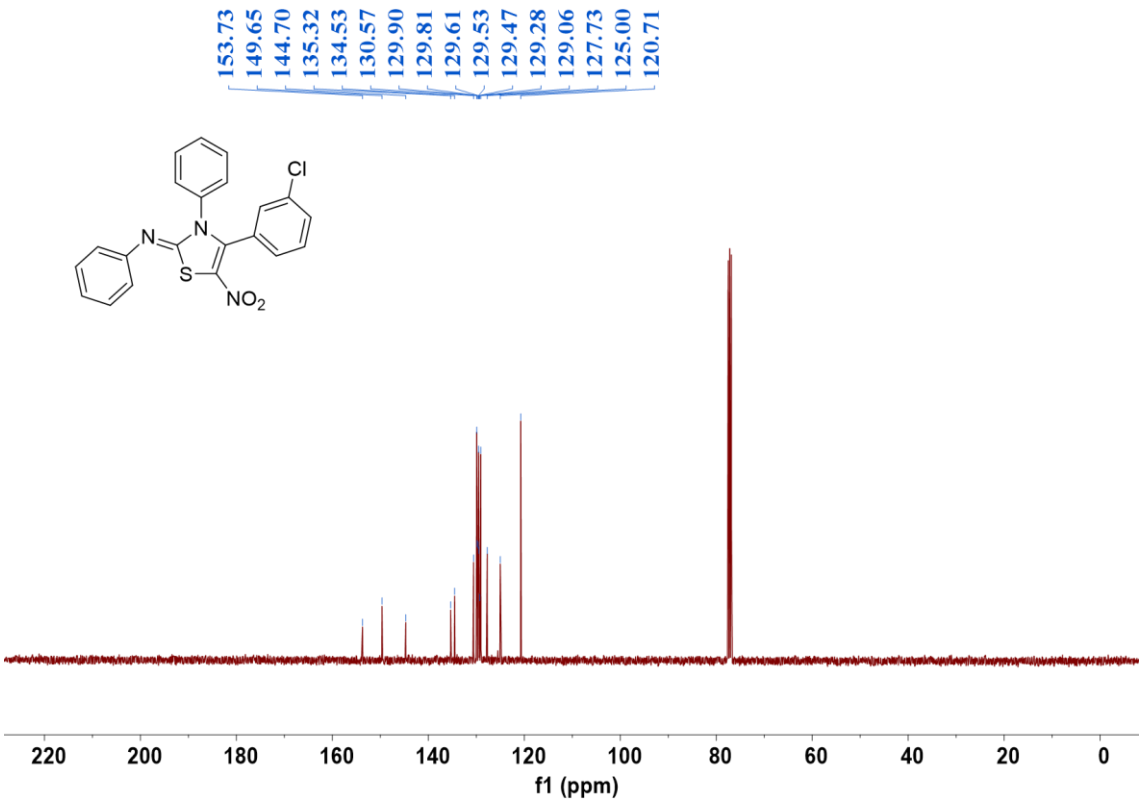
f1 (ppm)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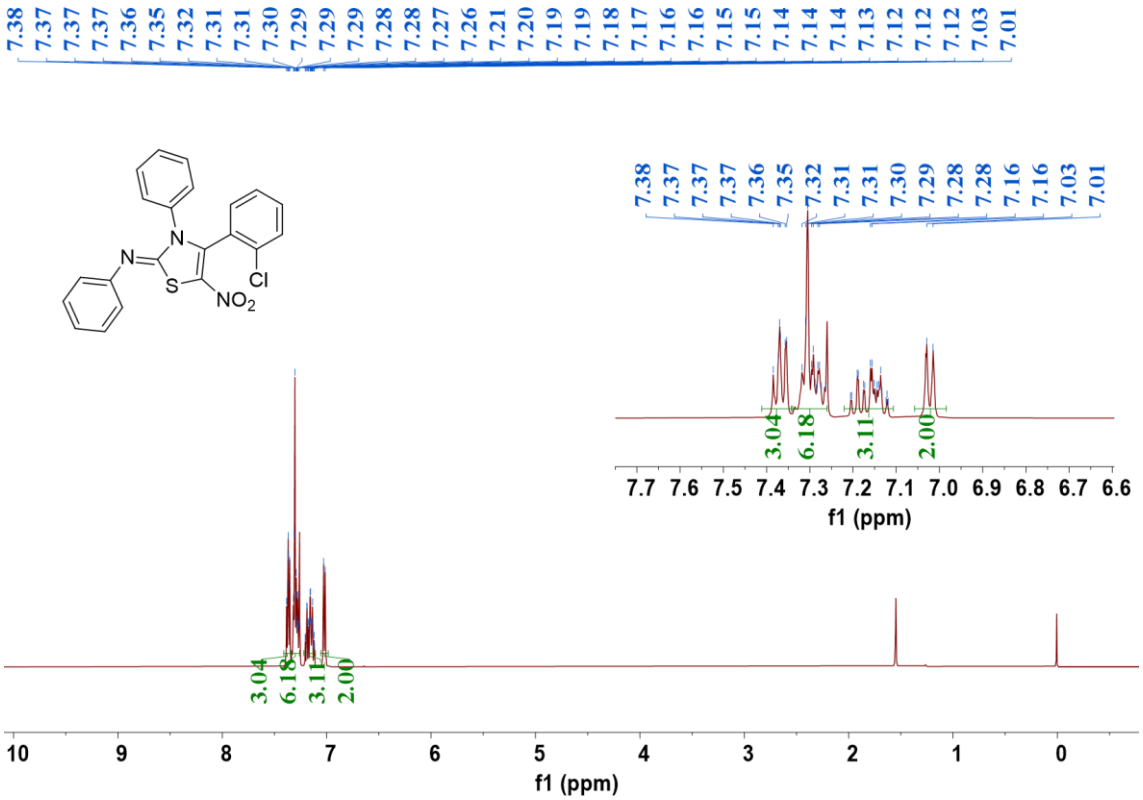
Cl
N
S
NO2
f1 (ppm)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S
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NO2
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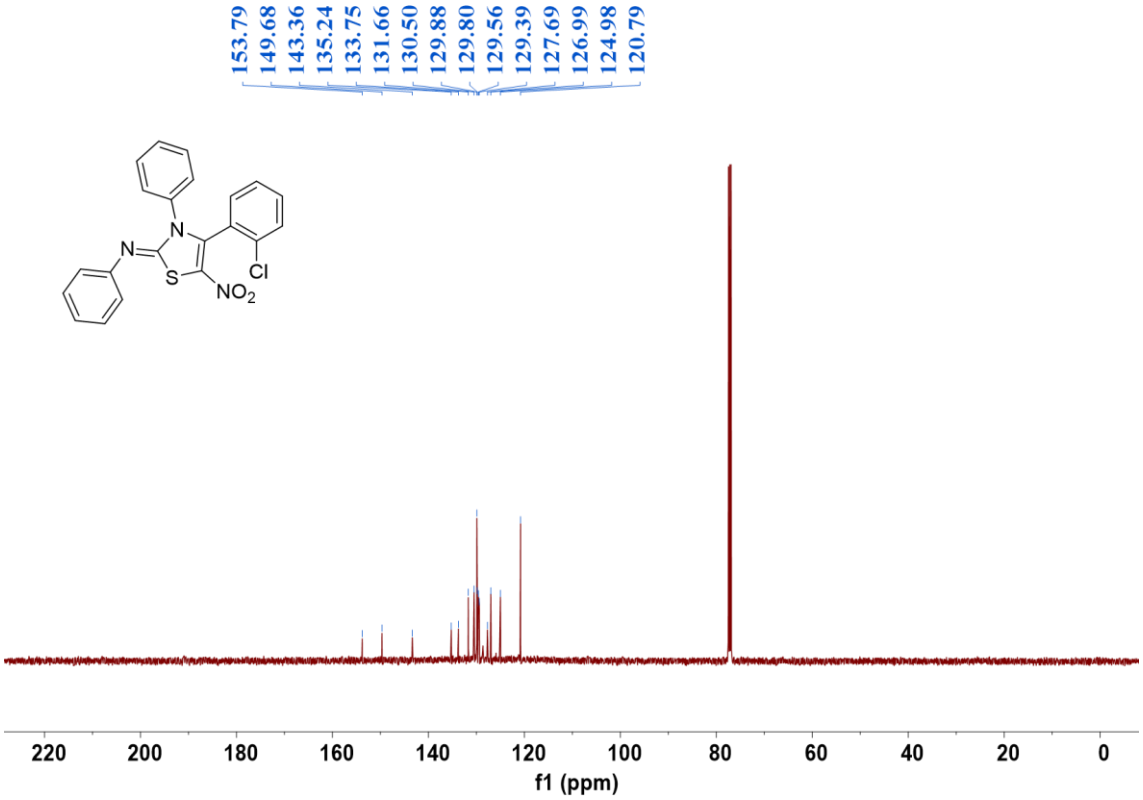
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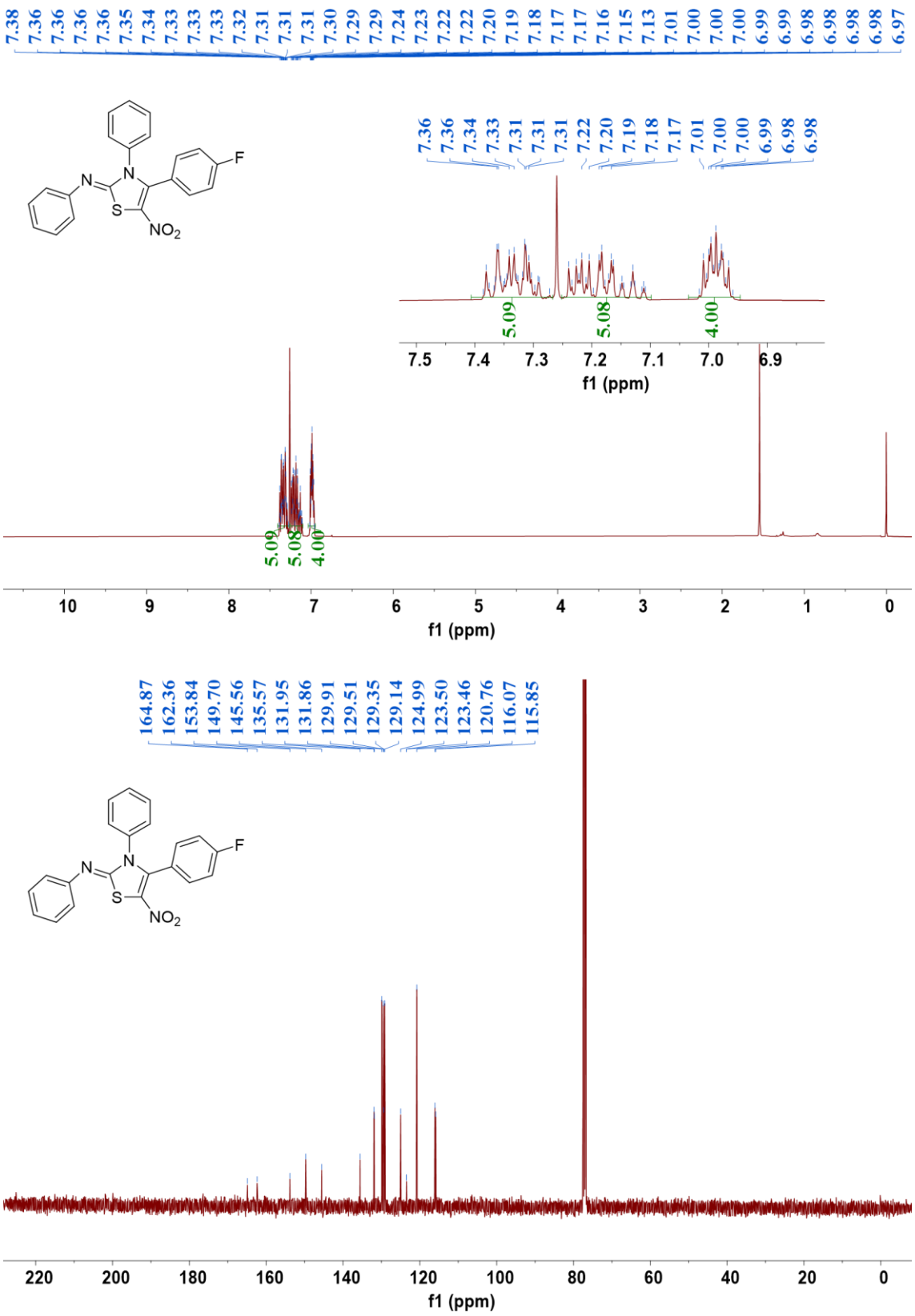
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F
N
S
NO2
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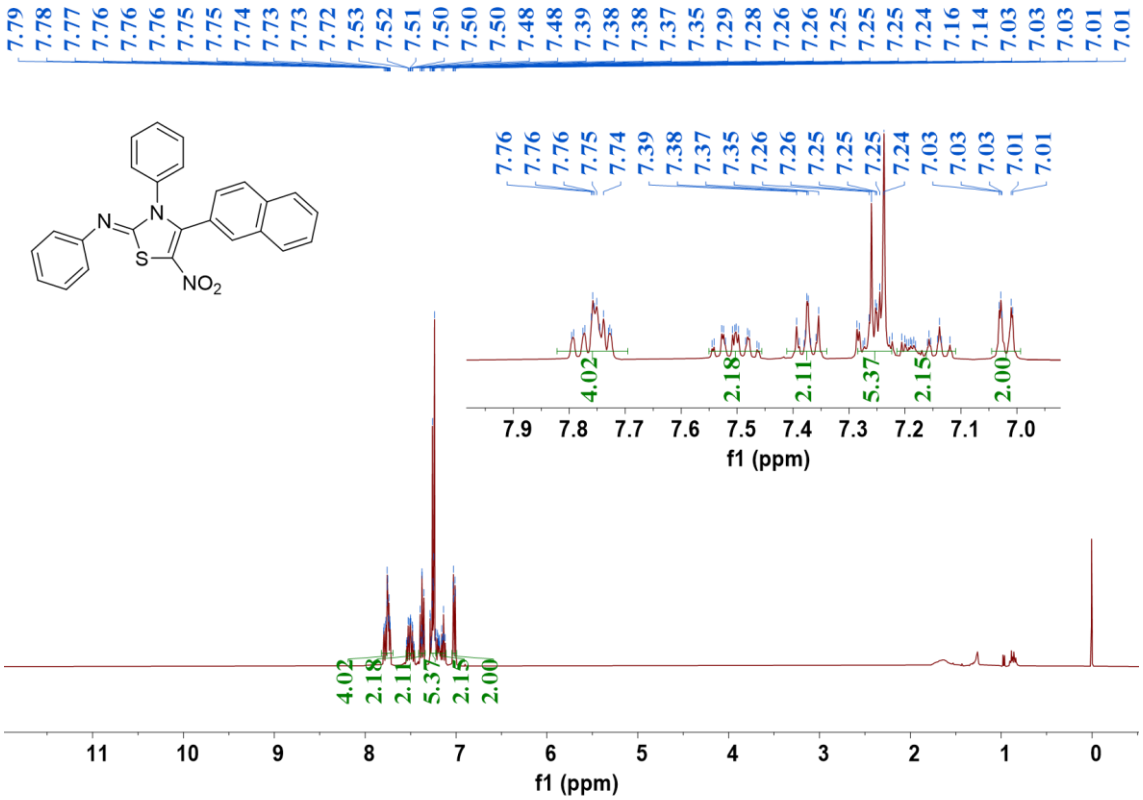
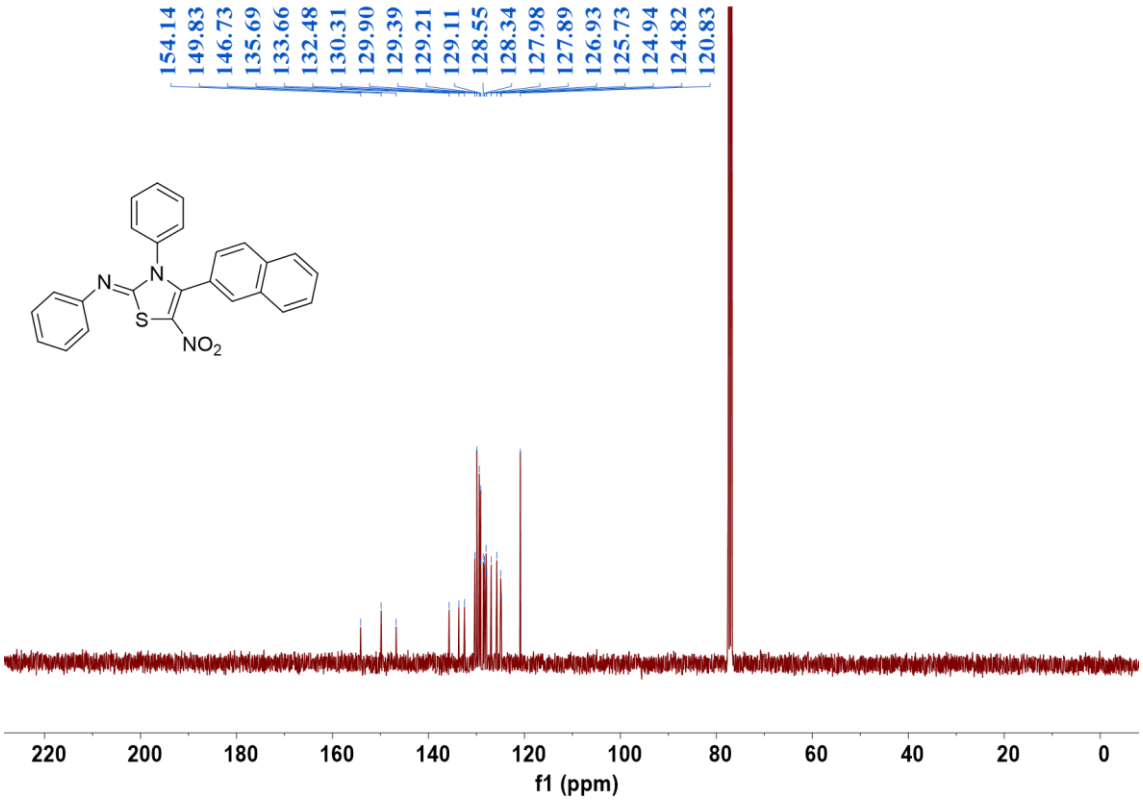
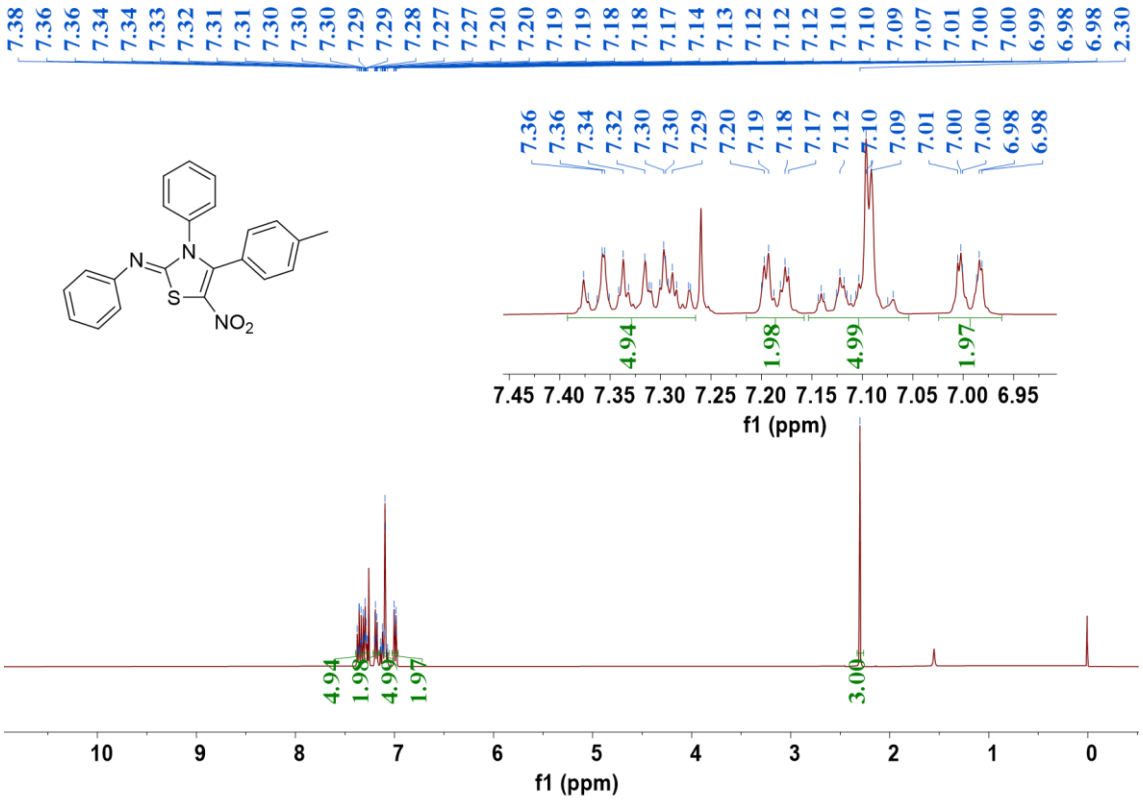
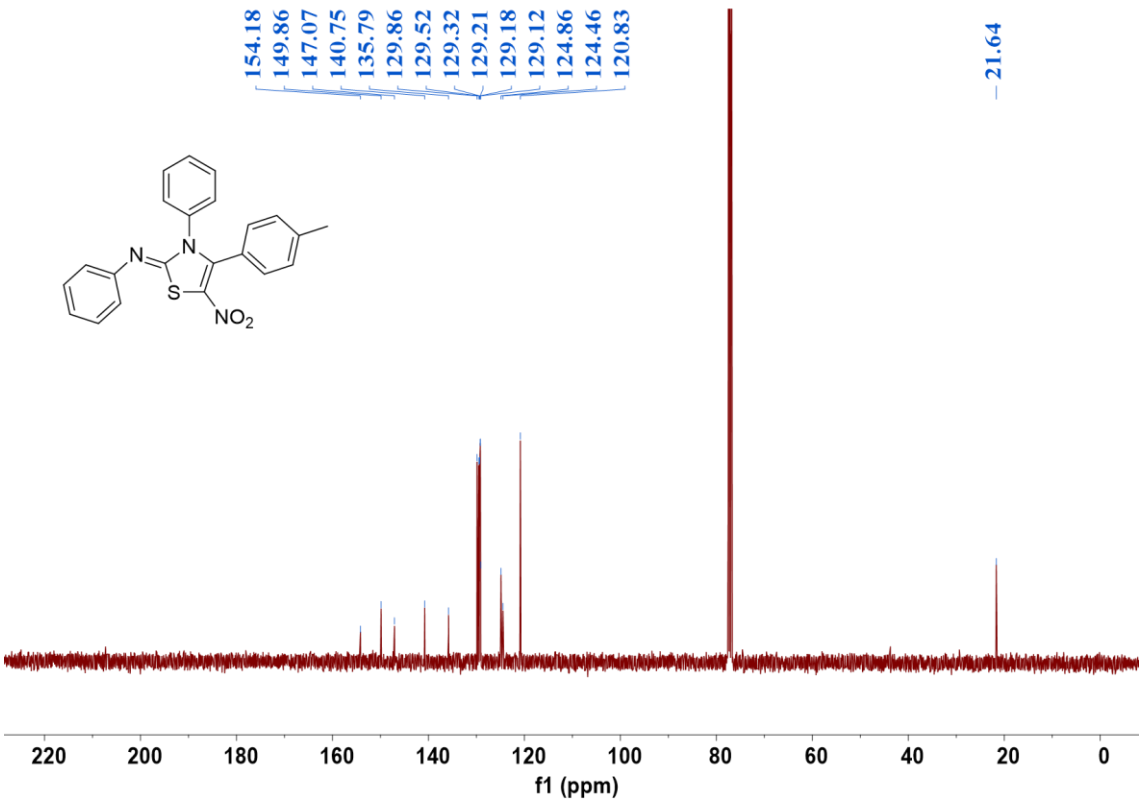
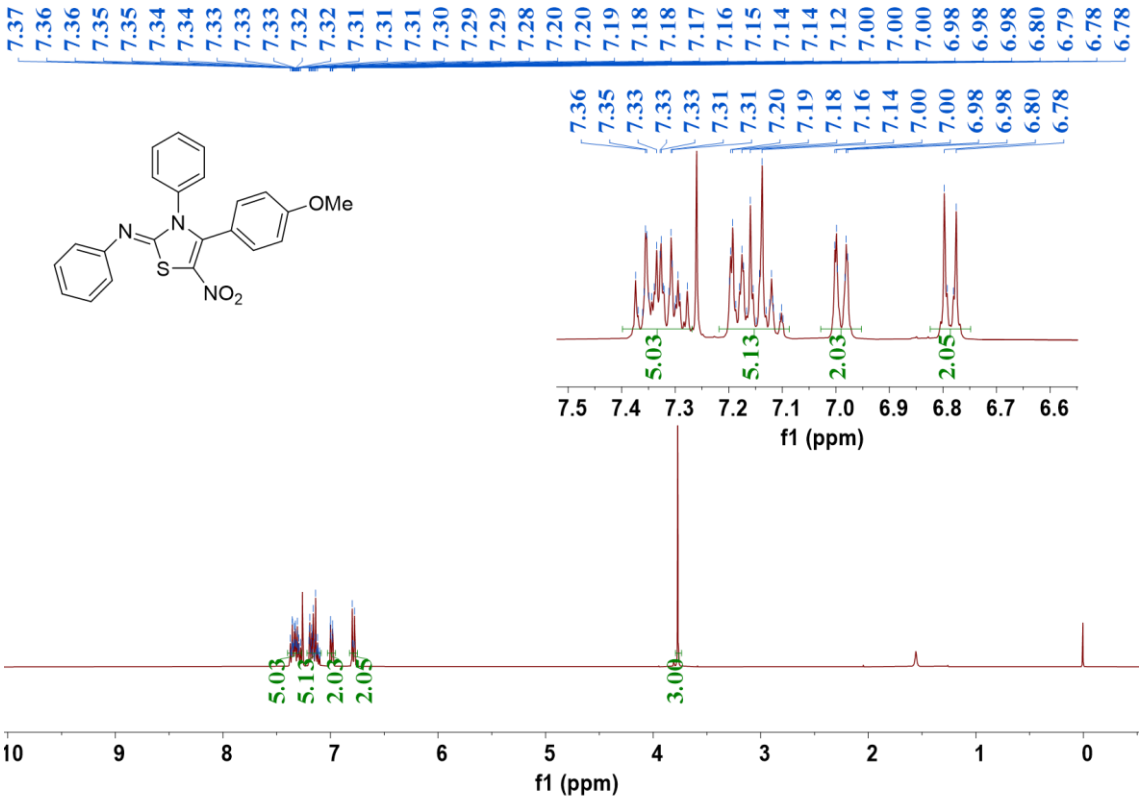
5.09
5.08
4.00
7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
5.09
5.08
4.00
10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)
164.87 162.36 153.84 149.70 145.56 135.57 131.95 131.86 129.91 129.51 129.35 129.14 124.99 123.50 123.46 120.76 116.07 115.85
F
N
S
NO2
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)


7.79 7.78 7.77 7.76 7.76 7.76 7.75 7.75 7.74 7.73 7.73 7.72 7.53 7.52 7.51 7.50 7.50 7.50 7.48 7.48 7.39 7.38 7.38 7.37 7.35 7.29 7.28 7.26 7.26 7.25 7.25 7.25 7.24 7.16 7.14 7.03 7.03 7.03 7.01 7.01
N
N
S
NO2
4.02 2.18 2.11 5.37 2.15 2.00
f1 (ppm)


154.14 149.83 146.73 135.69 133.66 132.48 130.31 129.90 129.39 129.21 129.11 128.55 128.34 127.98 127.89 126.93 125.73 124.94 124.82 120.83
N
N
S
NO2
f1 (ppm)


7.38 7.36 7.36 7.34 7.34 7.33 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.29 7.28 7.27 7.27 7.20 7.20 7.19 7.19 7.18 7.18 7.17 7.14 7.13 7.12 7.12 7.12 7.10 7.10 7.09 7.07 7.01 7.00 7.00 6.99 6.98 6.98 2.30
7.36 7.36 7.34 7.32 7.30 7.30 7.29 7.20 7.19 7.18 7.17 7.12 7.10 7.09 7.01 7.00 7.00 6.98 6.98
4.94 1.98 4.99 1.97
7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95
f1 (ppm)
4.94 1.98 4.99 1.97 3.00
10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


154.18 149.86 147.07 140.75 135.79 129.86 129.52 129.32 129.21 129.18 129.12 124.86 124.46 120.83
21.64
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)


7.37 7.36 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.31 7.30 7.29 7.29 7.28 7.20 7.20 7.19 7.18 7.18 7.17 7.16 7.15 7.14 7.14 7.12 7.00 7.00 7.00 6.98 6.98 6.98 6.80 6.79 6.78 6.78
OMe
N
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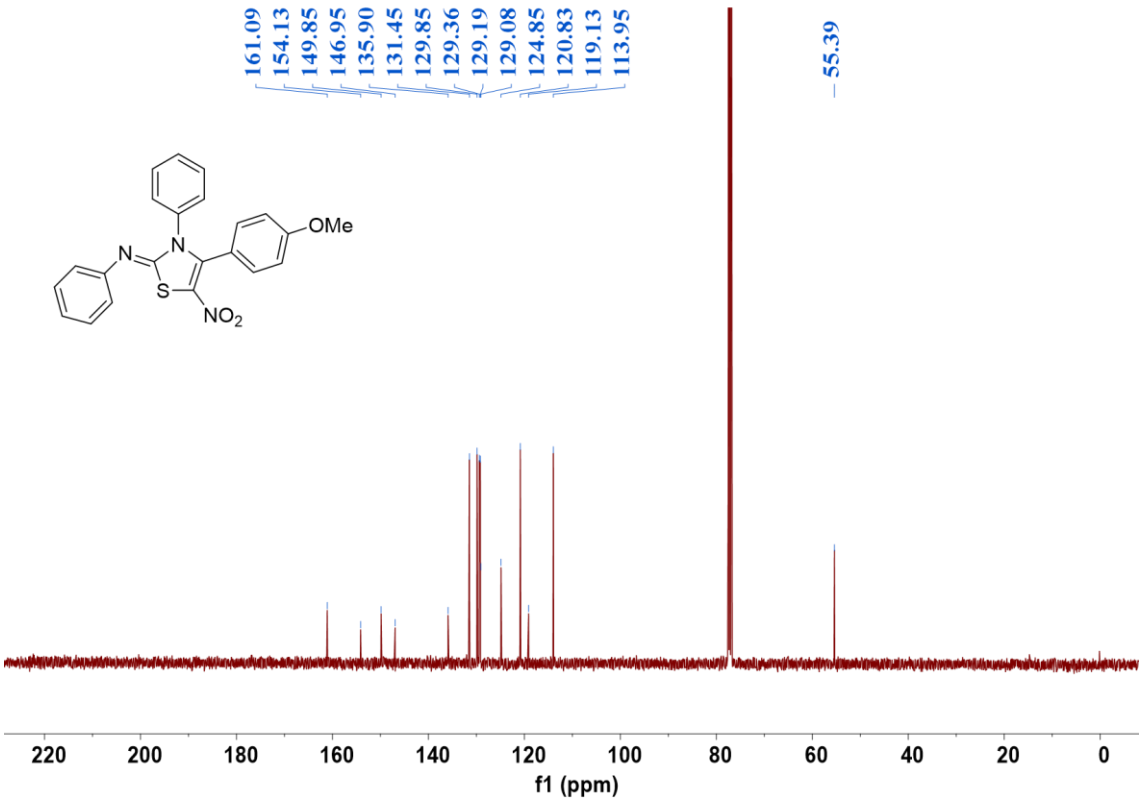
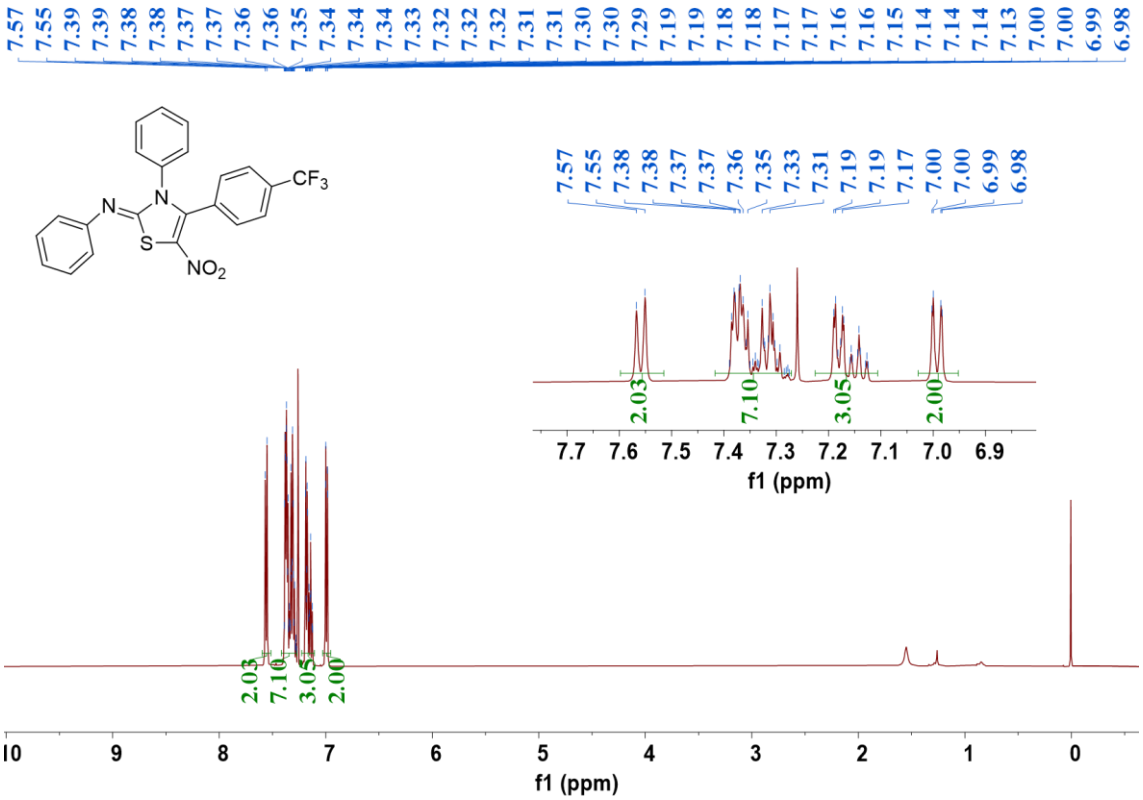
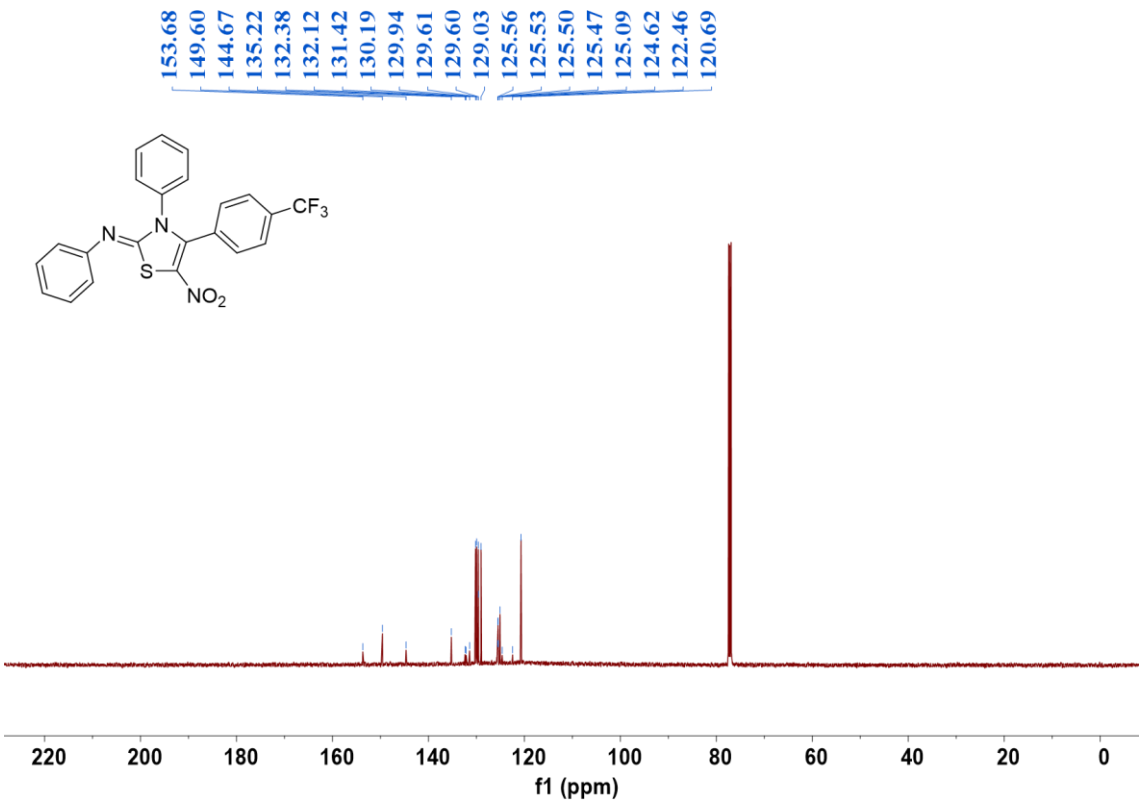
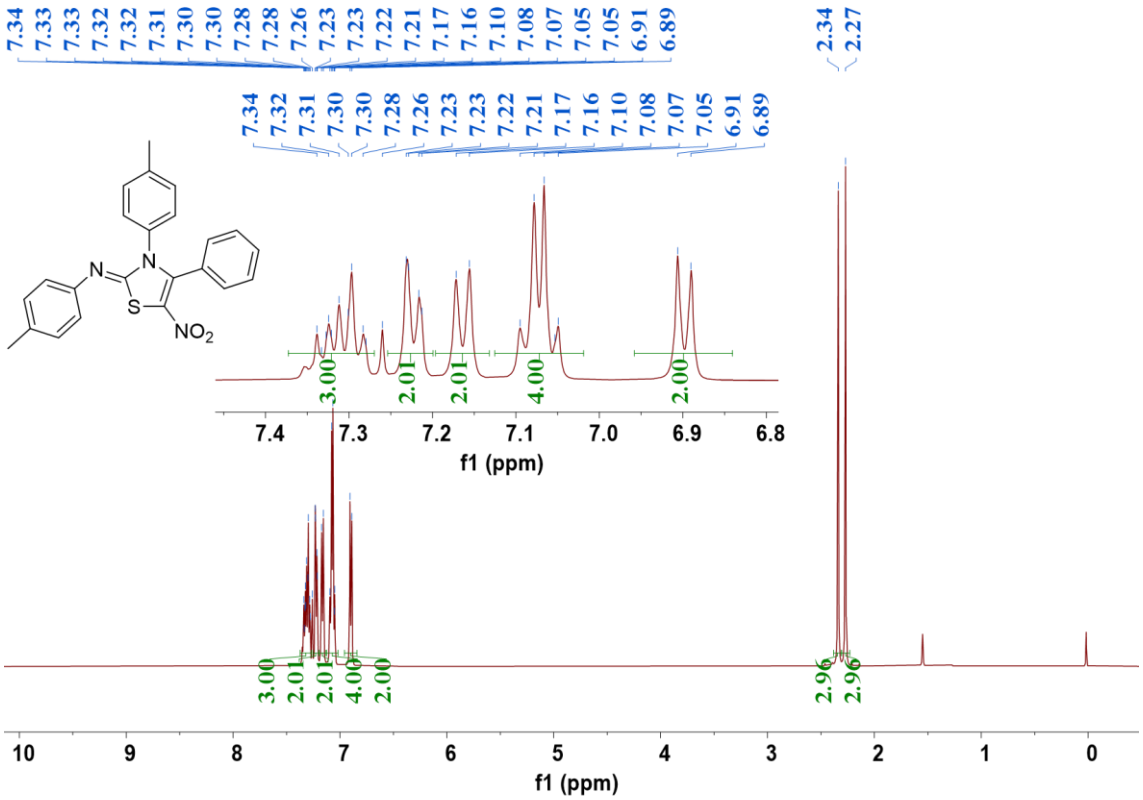
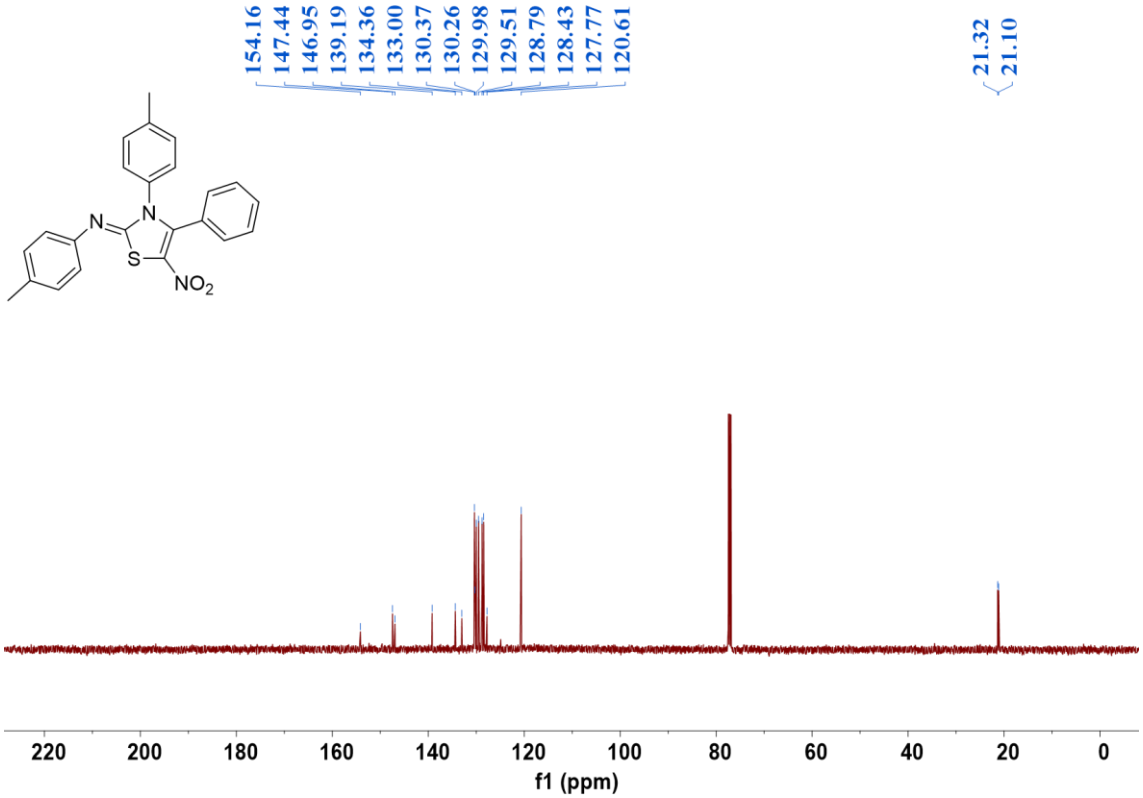
5.13
2.03
2.05
3.00
f1 (ppm)

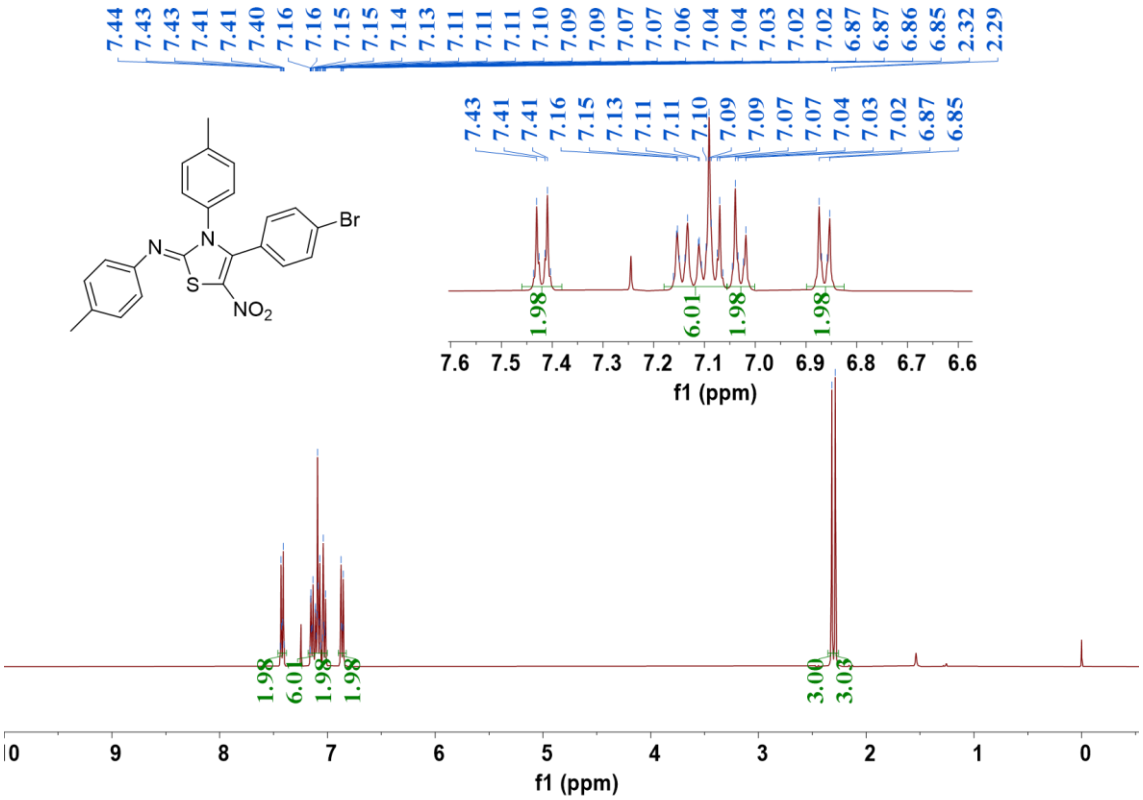

161.09 154.13 149.85 146.95 135.90 131.45 129.85 129.36 129.19 129.08 124.85 120.83 119.13 113.95
55.39
OMe
N
S
NO2
f1 (ppm)

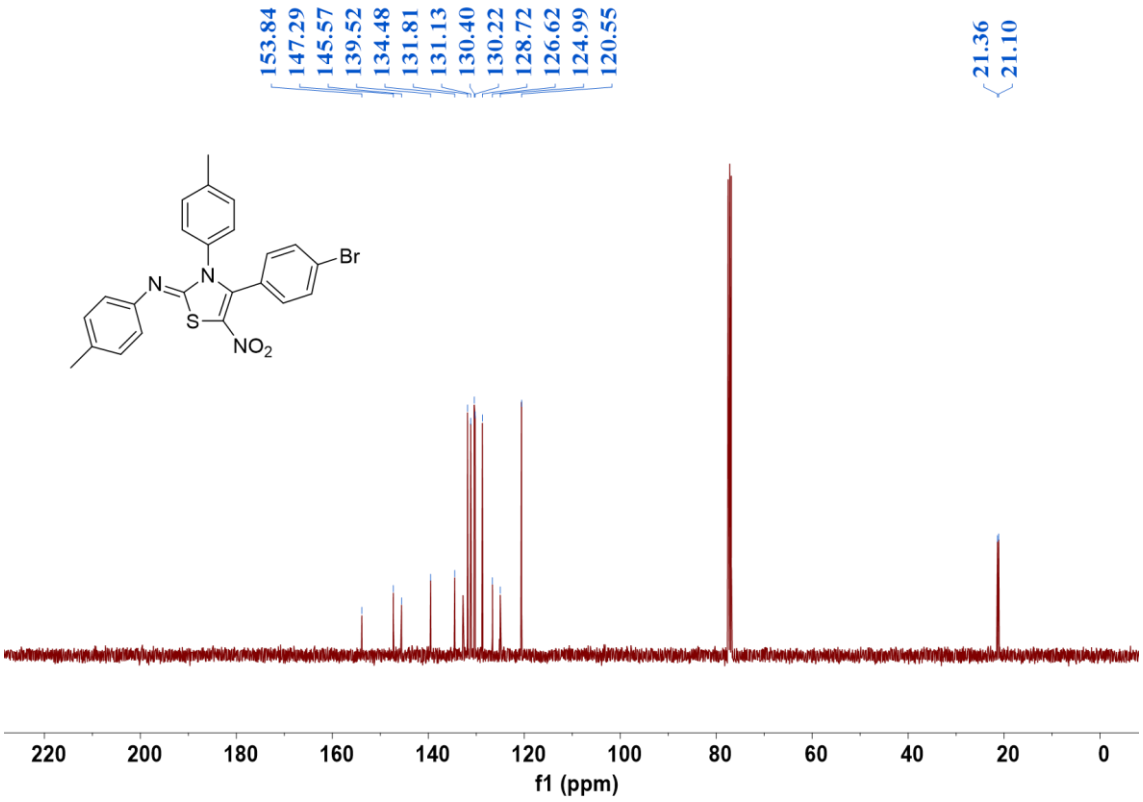

7.57 7.55 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.34 7.33 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.19 7.19 7.18 7.18 7.17 7.17 7.16 7.16 7.15 7.14 7.14 7.14 7.13 7.00 7.00 6.99 6.98
CF3
N
S
NO2
2.03 7.10 3.05 2.00
f1 (ppm)

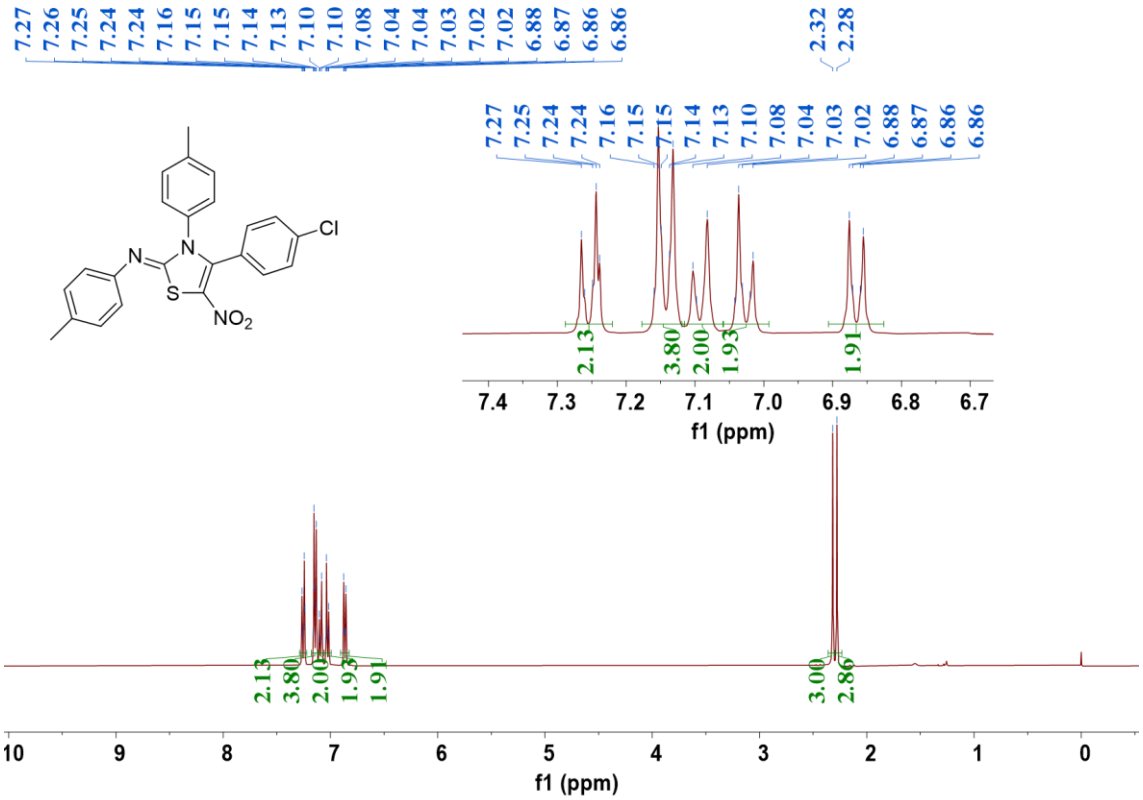

153.68 149.60 144.67 135.22 132.38 132.12 131.42 130.19 129.94 129.61 129.60 129.03 125.56 125.53 125.50 125.47 125.09 124.62 122.46 120.69
CF3
N
S
NO2
f1 (ppm)

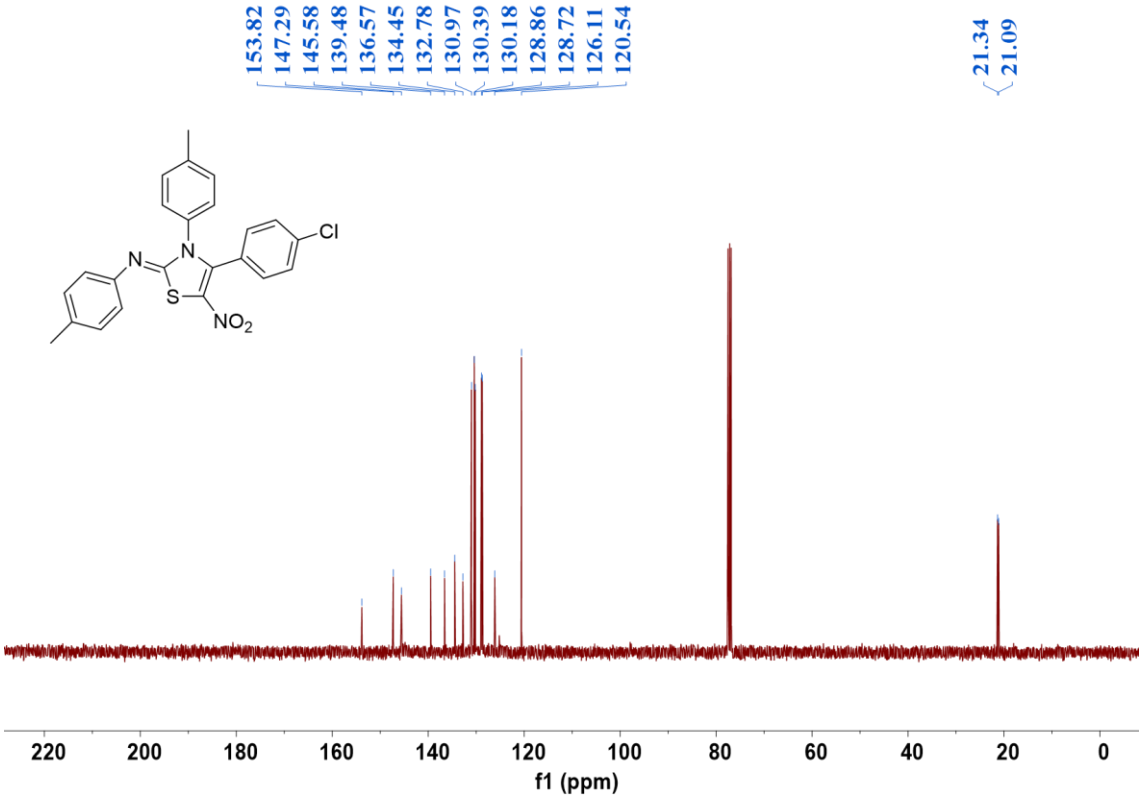

7.34 7.33 7.33 7.32 7.32 7.31 7.30 7.30 7.28 7.28 7.26 7.23 7.23 7.22 7.21 7.17 7.16 7.10 7.08 7.07 7.05 7.05 6.91 6.89
2.34 2.27
7.34 7.32 7.31 7.30 7.30 7.28 7.26 7.23 7.23 7.22 7.21 7.17 7.16 7.10 7.08 7.07 7.05 6.91 6.89
N
S
NO2
3.00 2.01 2.01 4.00 2.00
7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
3.00 2.01 2.01 4.00 2.00
2.96 2.96
10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

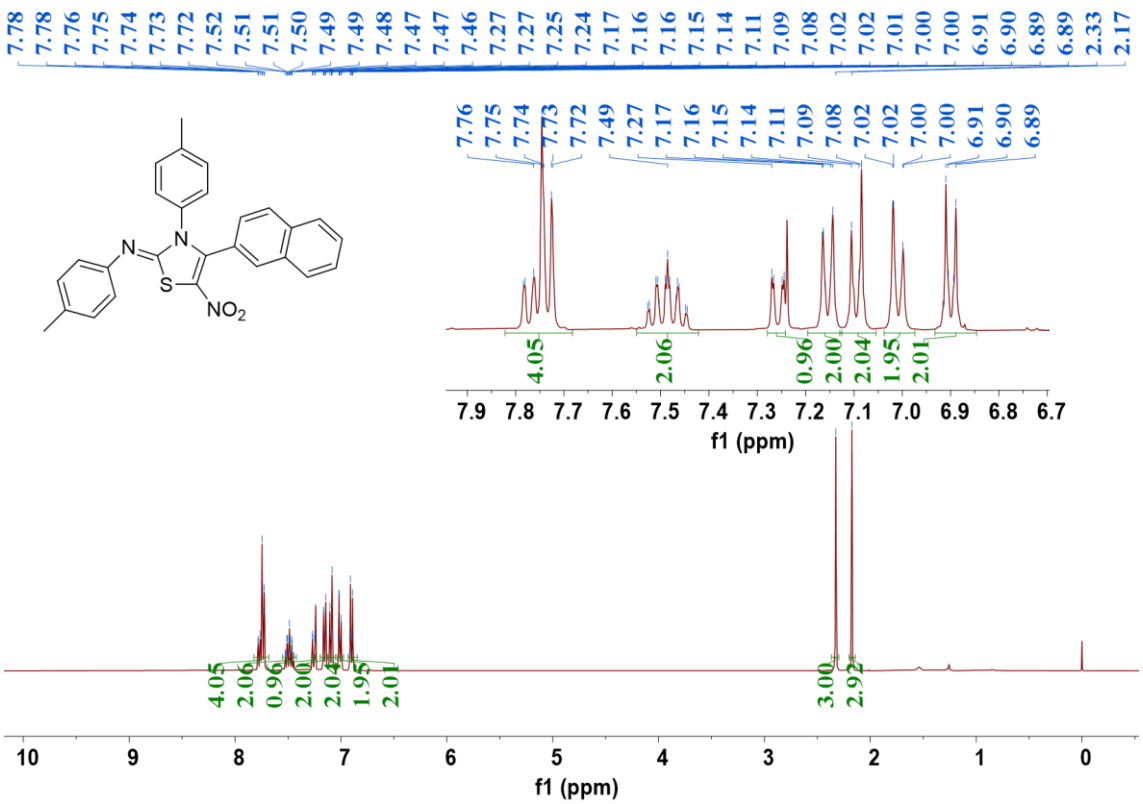

154.16 147.44 146.95 139.19 134.36 133.00 130.37 130.26 129.98 129.51 128.79 128.43 127.77 120.61
21.32 21.10
N
S
NO2
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

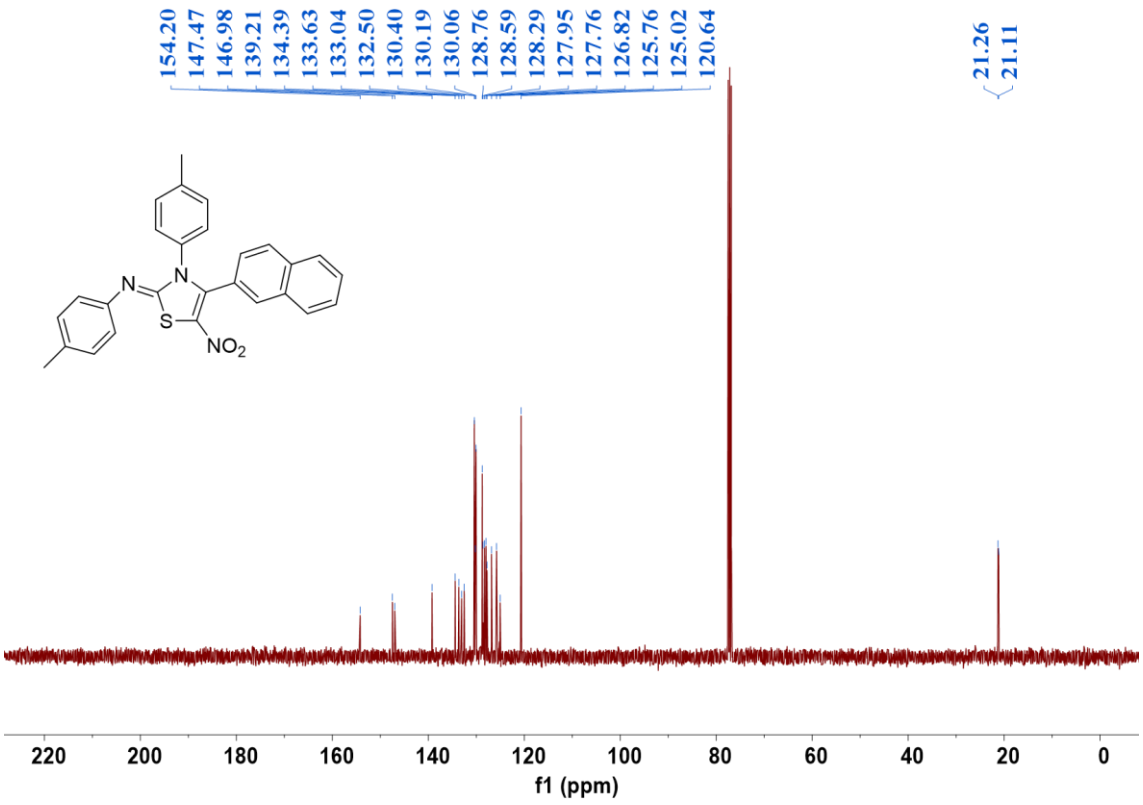

7.44 7.43 7.43 7.41 7.41 7.40 7.16 7.16 7.15 7.15 7.14 7.13 7.11 7.11 7.11 7.10 7.09 7.09 7.07 7.07 7.06 7.04 7.04 7.03 7.02 7.02 6.87 6.87 6.86 6.85 2.32 2.29
Br
N
S
NO2
1.98 6.01 1.98 1.98 3.00 3.03
f1 (ppm)


153.84 147.29 145.57 139.52 134.48 131.81 131.13 130.40 130.22 128.72 126.62 124.99 120.55
21.36 21.10
Br
N
S
NO2
f1 (ppm)


7.27 7.26 7.25 7.24 7.24 7.16 7.15 7.15 7.14 7.13 7.10 7.10 7.08 7.04 7.04 7.03 7.02 7.02 6.88 6.87 6.86 6.86
2.32 2.28
Cl
N
S
NO2
2.13 3.80 2.00 1.93 1.91
3.00 2.86
f1 (ppm)


153.82 147.29 145.58 139.48 136.57 134.45 132.78 130.97 130.39 130.18 128.86 128.72 126.11 120.54
21.34 21.09
Cl
N
S
NO2
f1 (ppm)


7.78 7.78 7.76 7.75 7.74 7.73 7.72 7.52 7.51 7.51 7.50 7.49 7.49 7.48 7.47 7.47 7.46 7.27 7.27 7.25 7.24 7.17 7.16 7.16 7.15 7.14 7.11 7.09 7.08 7.02 7.02 7.01 7.00 7.00 6.91 6.90 6.89 6.89 2.33 2.17
7.76 7.75 7.74 7.73 7.72 7.49 7.27 7.17 7.16 7.15 7.14 7.11 7.09 7.08 7.02 7.02 7.00 7.00 6.91 6.90 6.89
4.05 2.06 0.96 2.00 2.04 1.95 2.01
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
4.05 2.06 0.96 2.00 2.04 1.95 2.01 3.00 2.92
10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)
N
S
NO2


154.20 147.47 146.98 139.21 134.39 133.63 133.04 132.50 130.40 130.19 130.06 128.76 128.59 128.29 127.95 127.76 126.82 125.76 125.02 120.64
21.26 21.11
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)
N
S
NO2