molecules

MDPI

Communication

A Concise Synthesis of Pyrrole-Based Drug Candidates from α-Hydroxyketones, 3-Oxobutanenitrile, and Anilines

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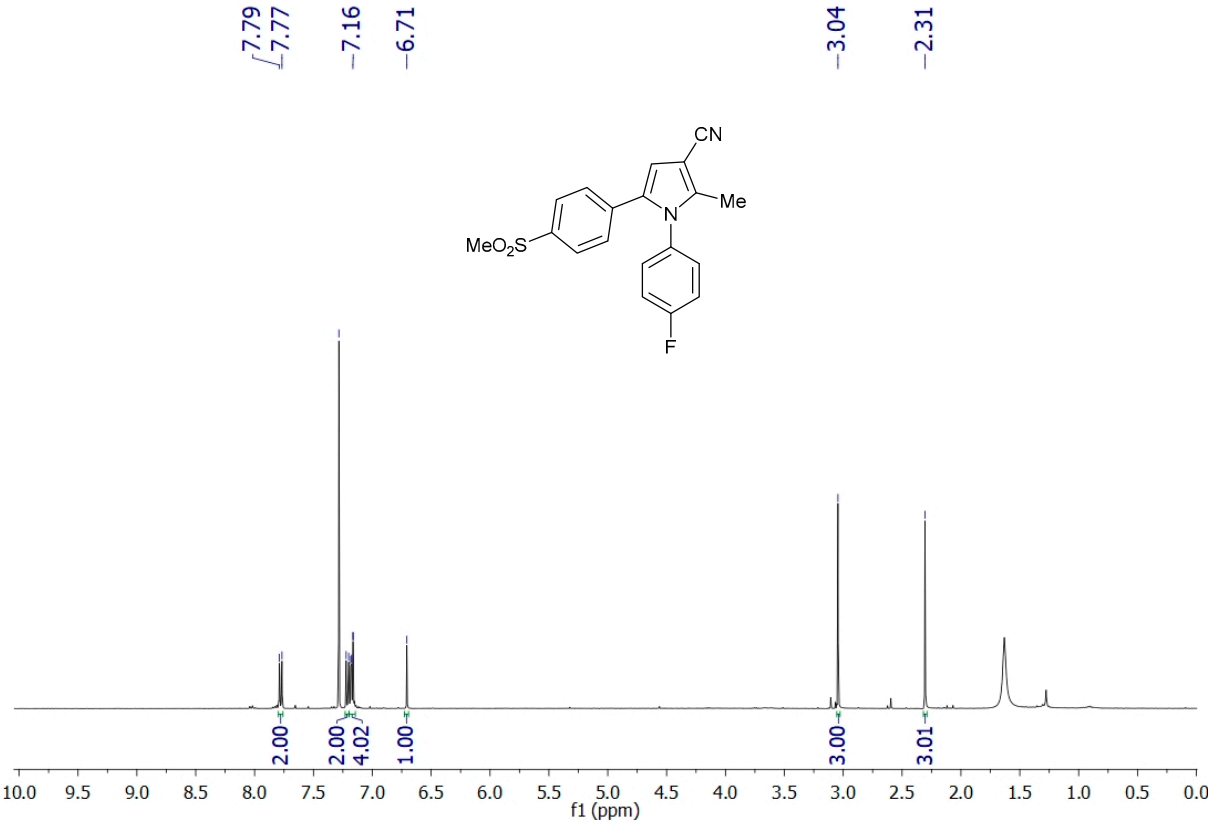
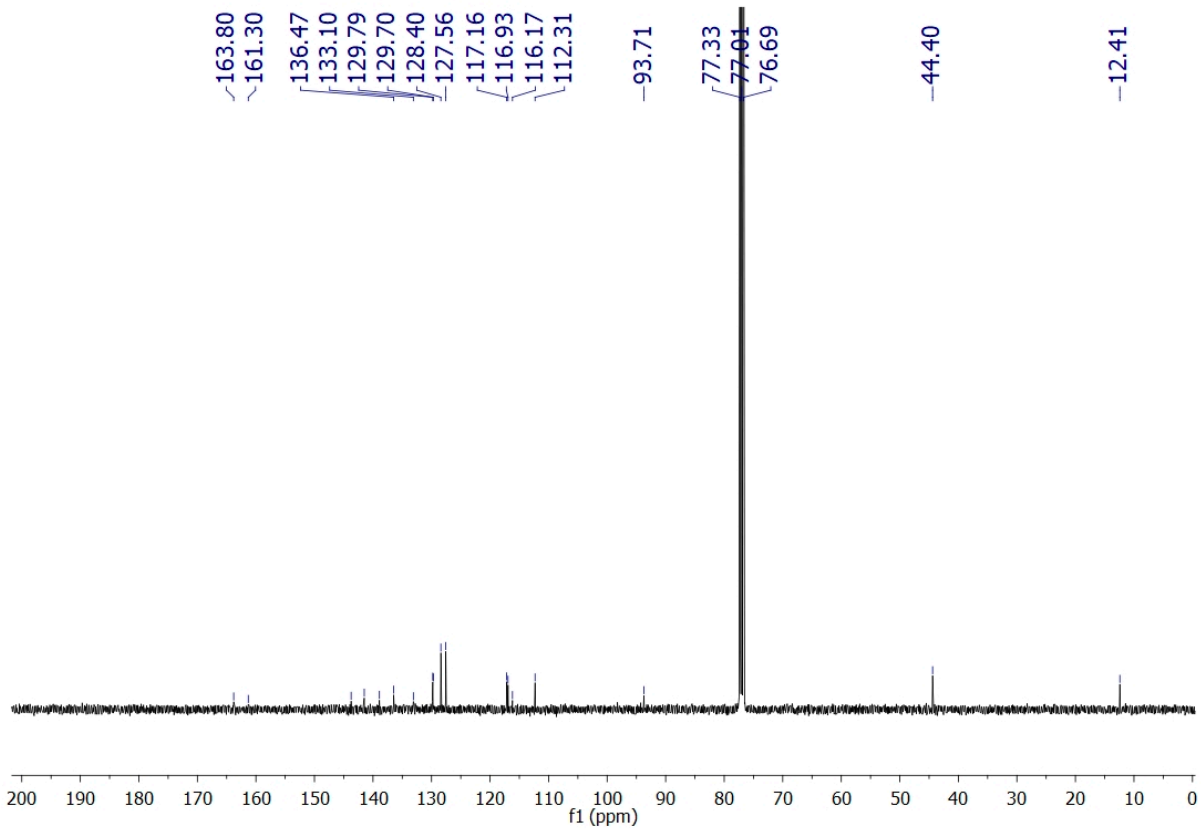
1.1. H NMR and ^{13}C NMR spectra

1-(4-Fluorophenyl)-2-methyl-5-(4-(methylsulfonyl)phenyl)-1*H*-pyrrole-3-carbonitrile **1a**

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136.47
133.10
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93.71
77.33
77.01
76.69
44.40
12.41
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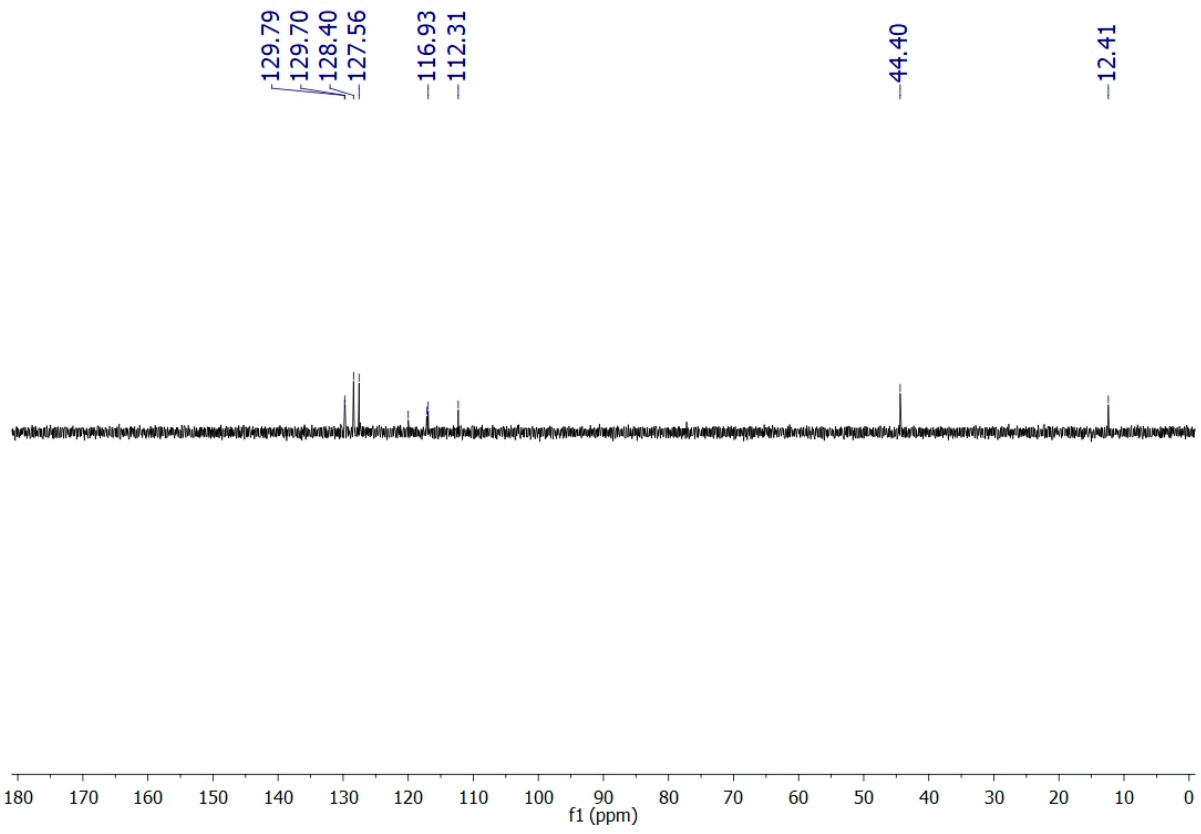
f1 (ppm)


129.79
129.70
128.40
127.56
116.93
112.31
44.40
12.41
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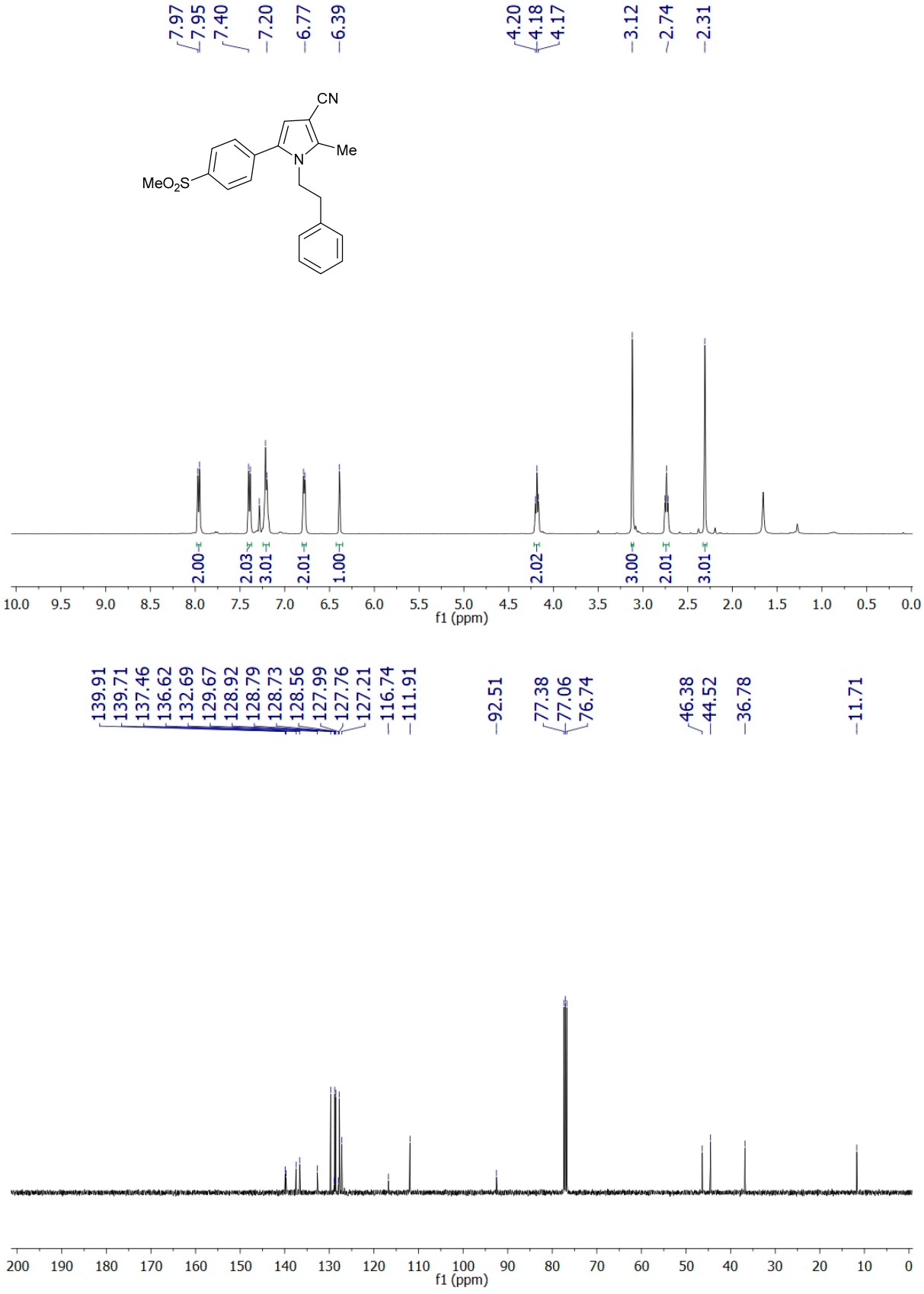
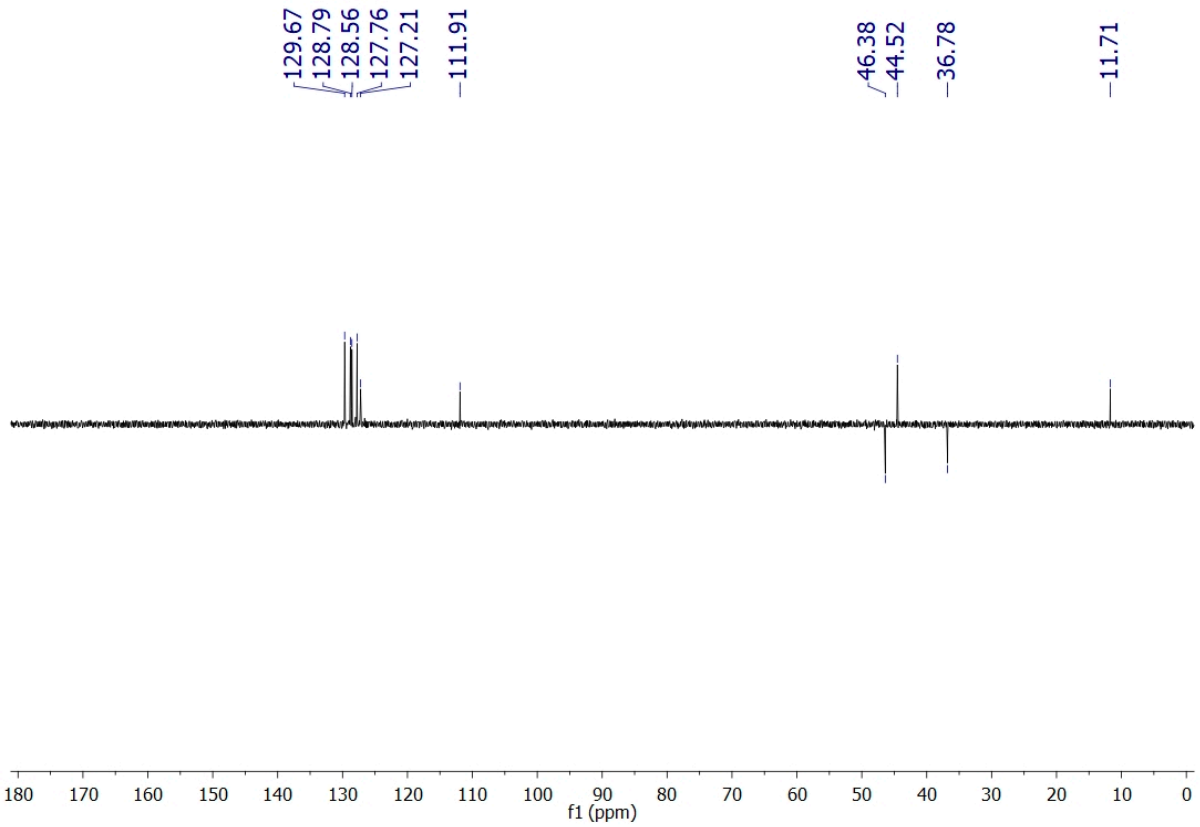
f1 (ppm)

2-Methyl-5-(4-(methylsulfonyl)phenyl)-1-phenethyl-1*H*-pyrrole-3-carbonitrile **9**

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128.79
128.56
127.76
127.21
111.91
46.38
44.52
36.78
11.71
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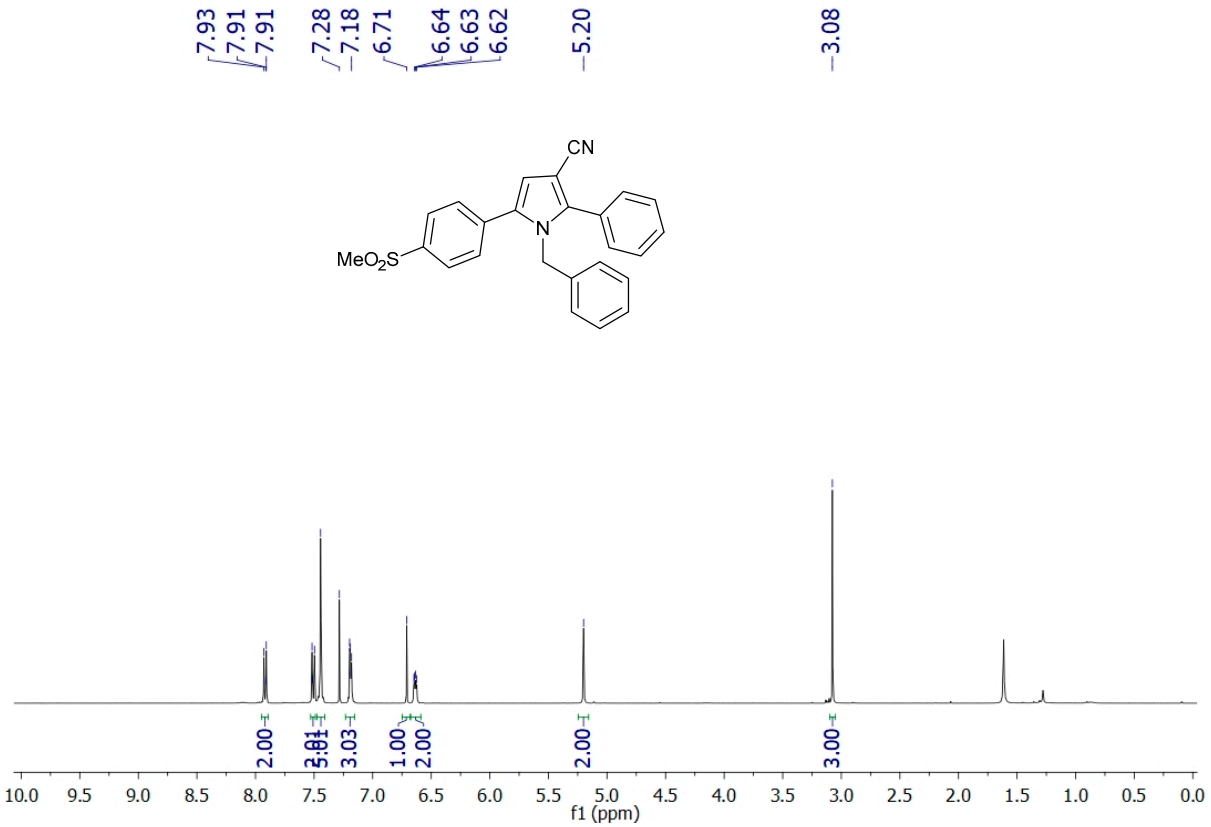
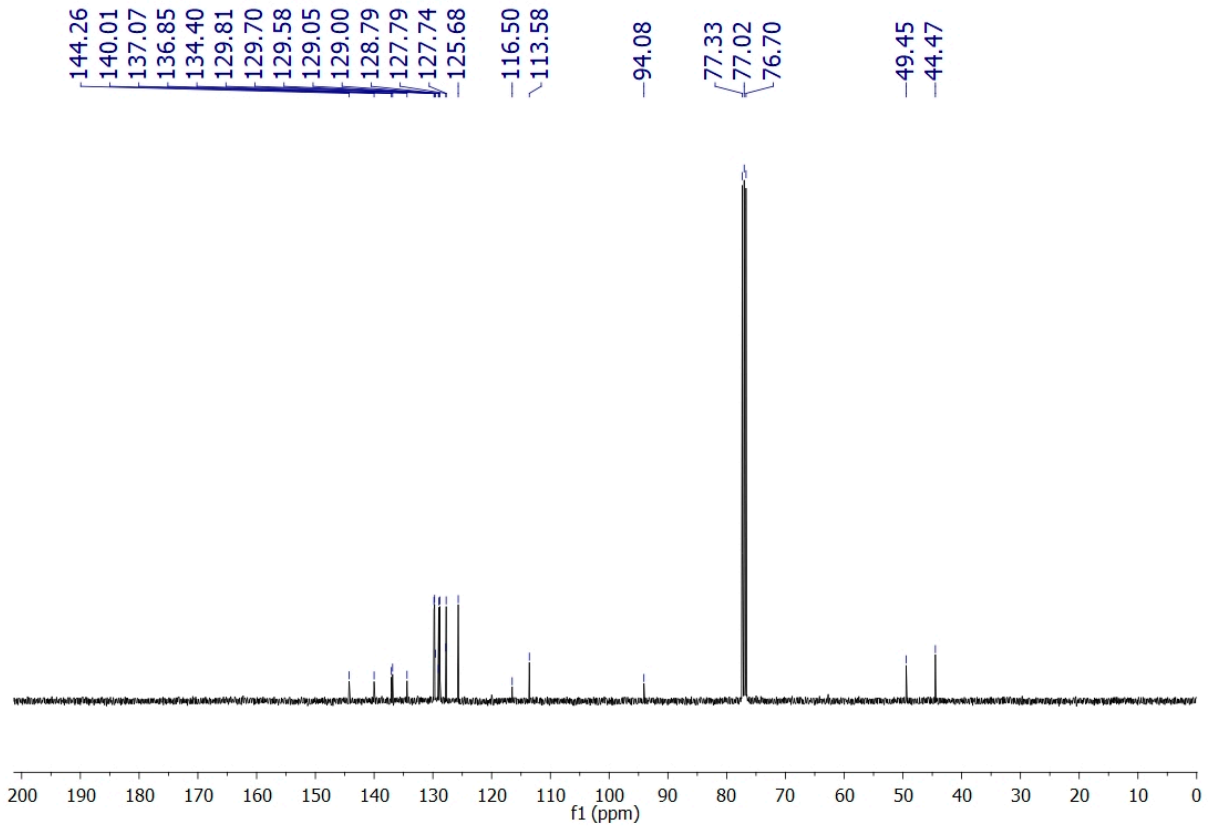
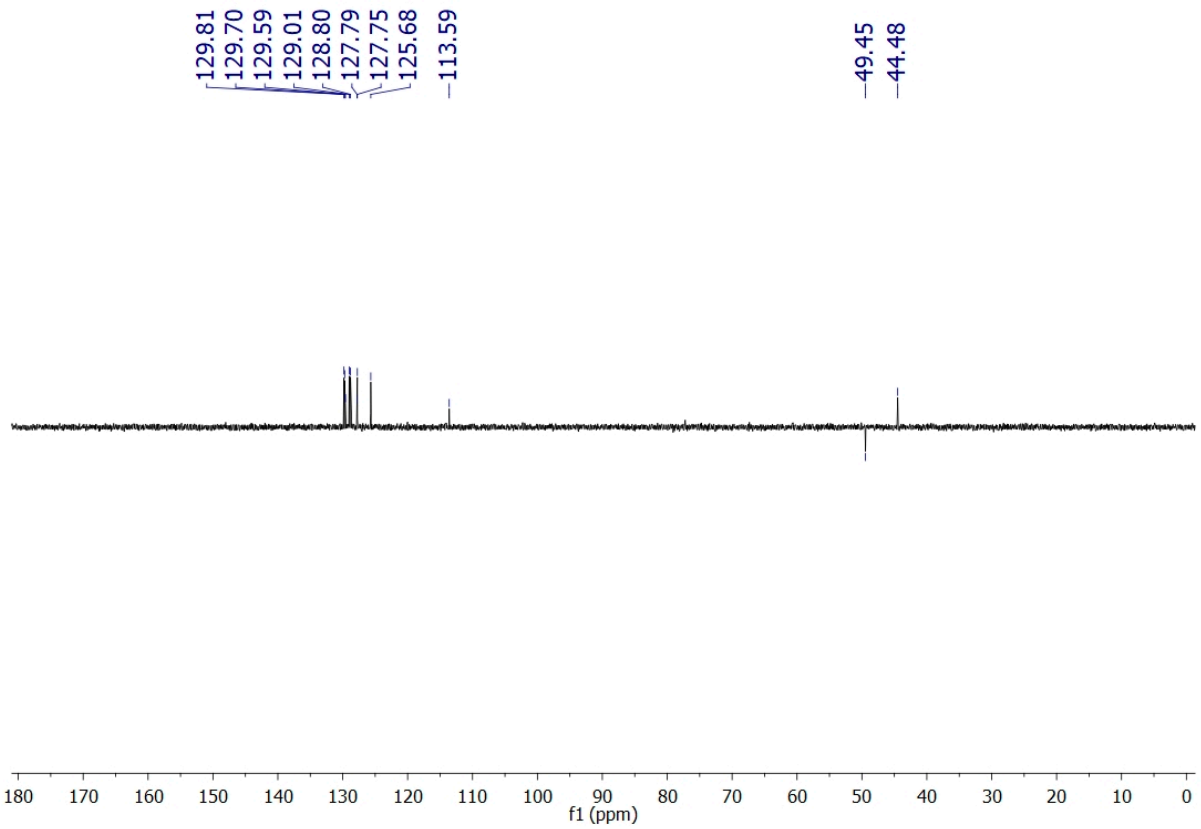
f1 (ppm)

1-Benzyl-5-(4-(methylsulfonyl)phenyl)-2-phenyl-1*H*-pyrrole-3-carbonitrile **10**



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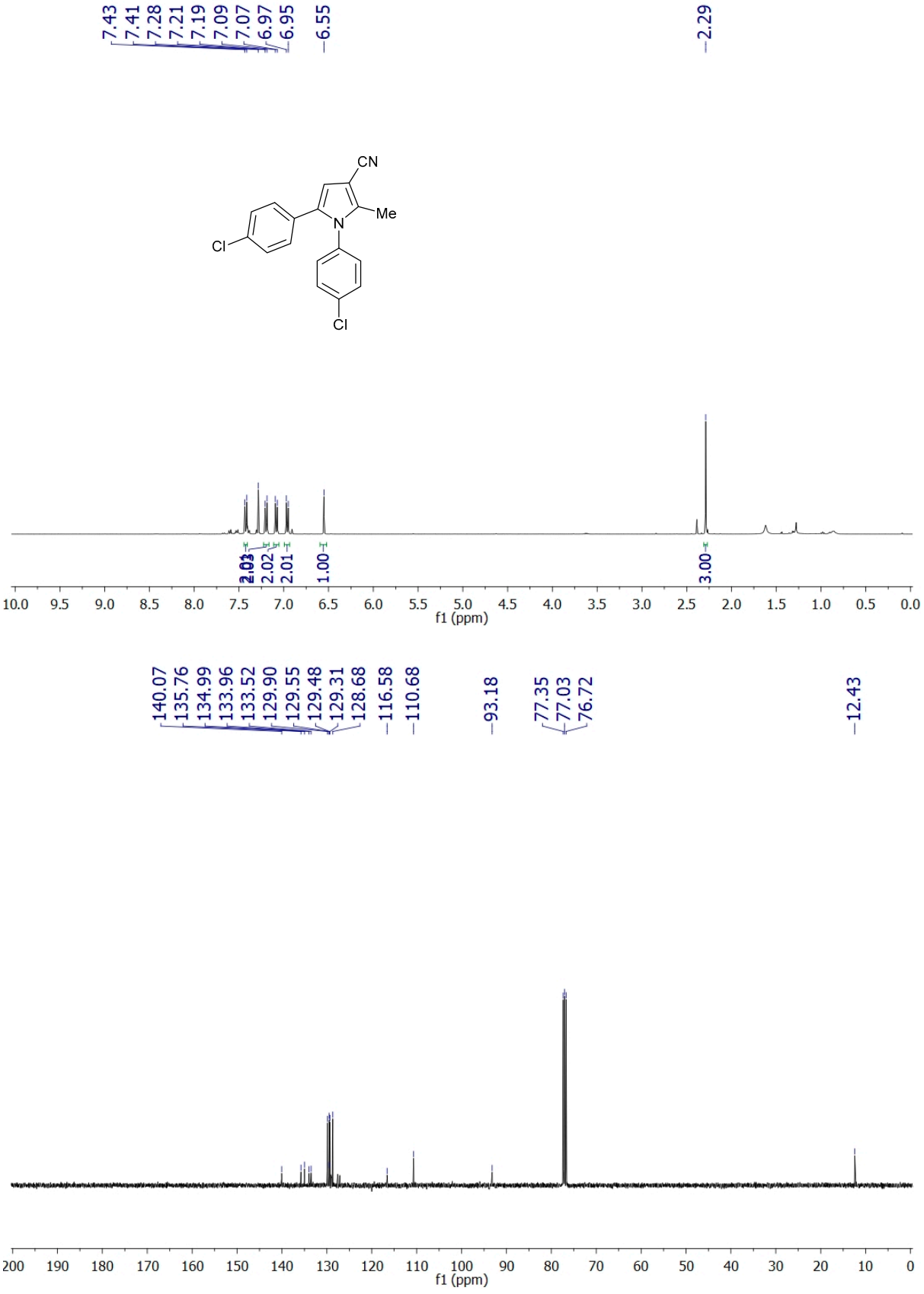
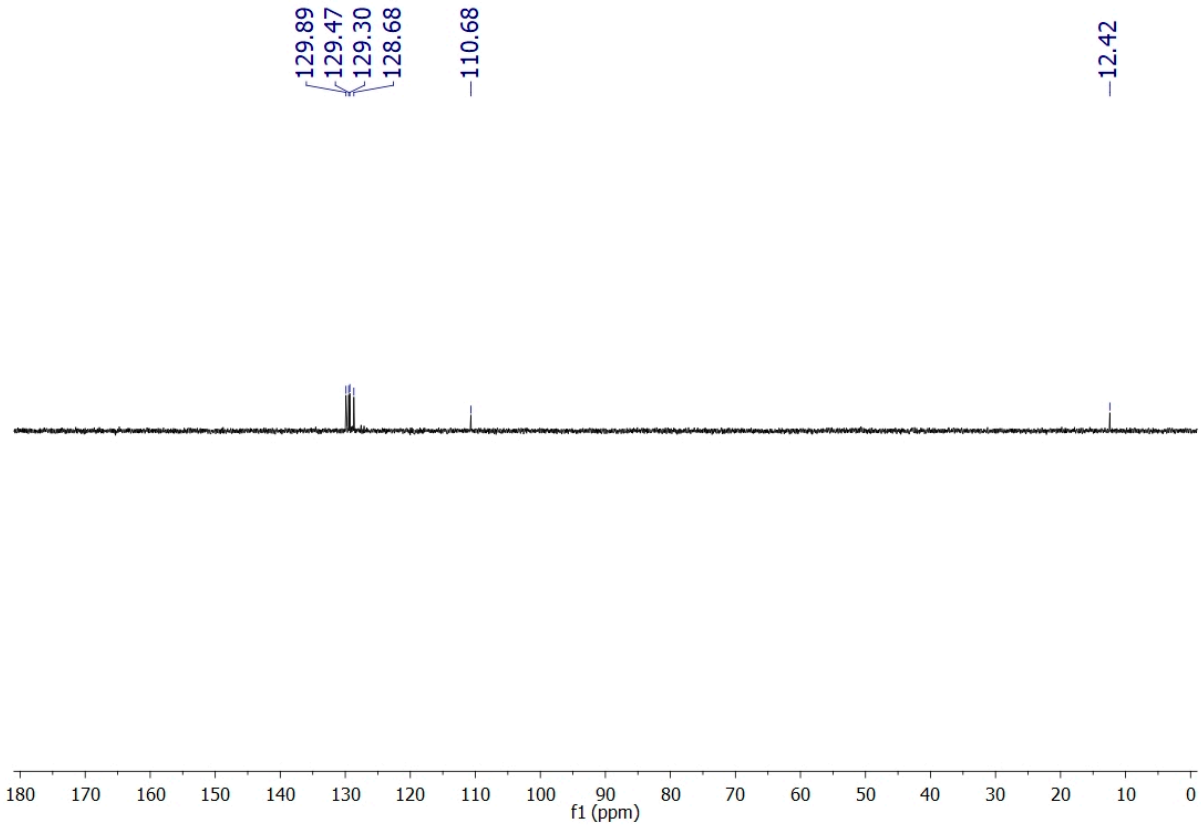
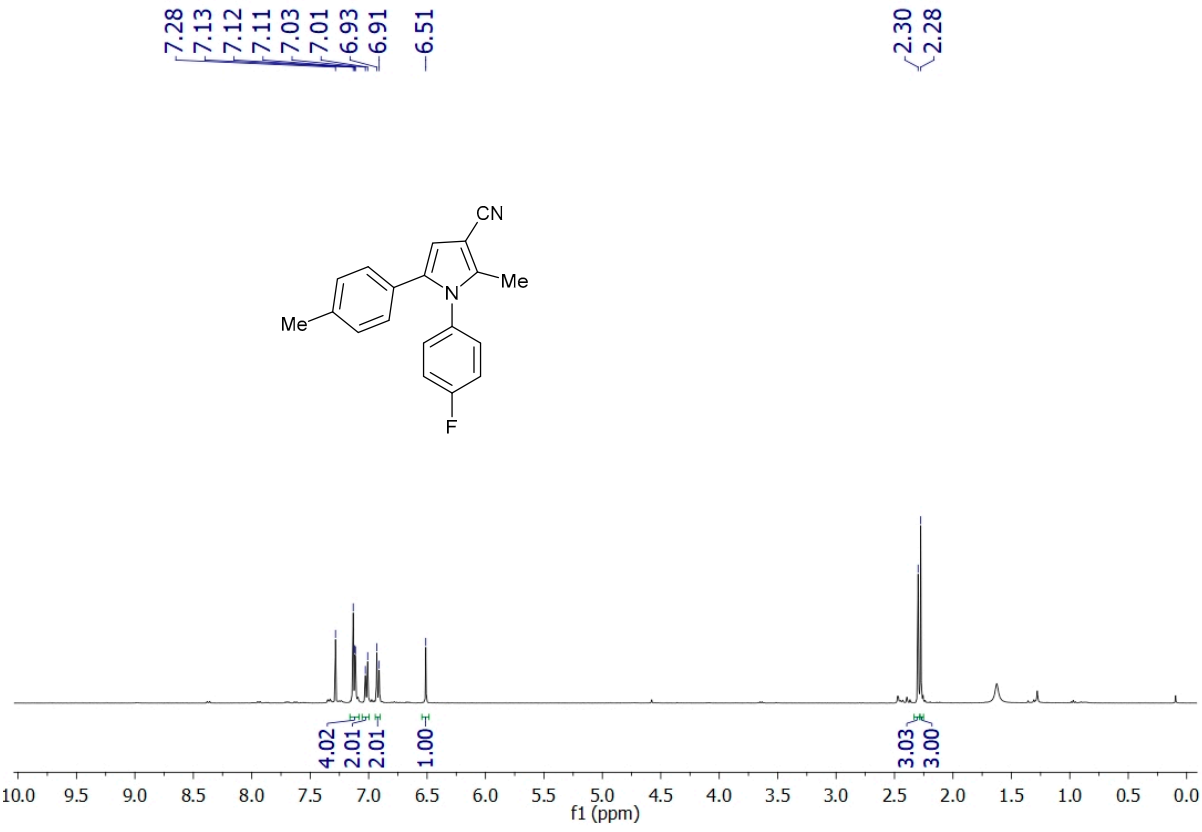
129.59
129.01
128.80
127.79
127.75
125.68
113.59
49.45
44.48
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

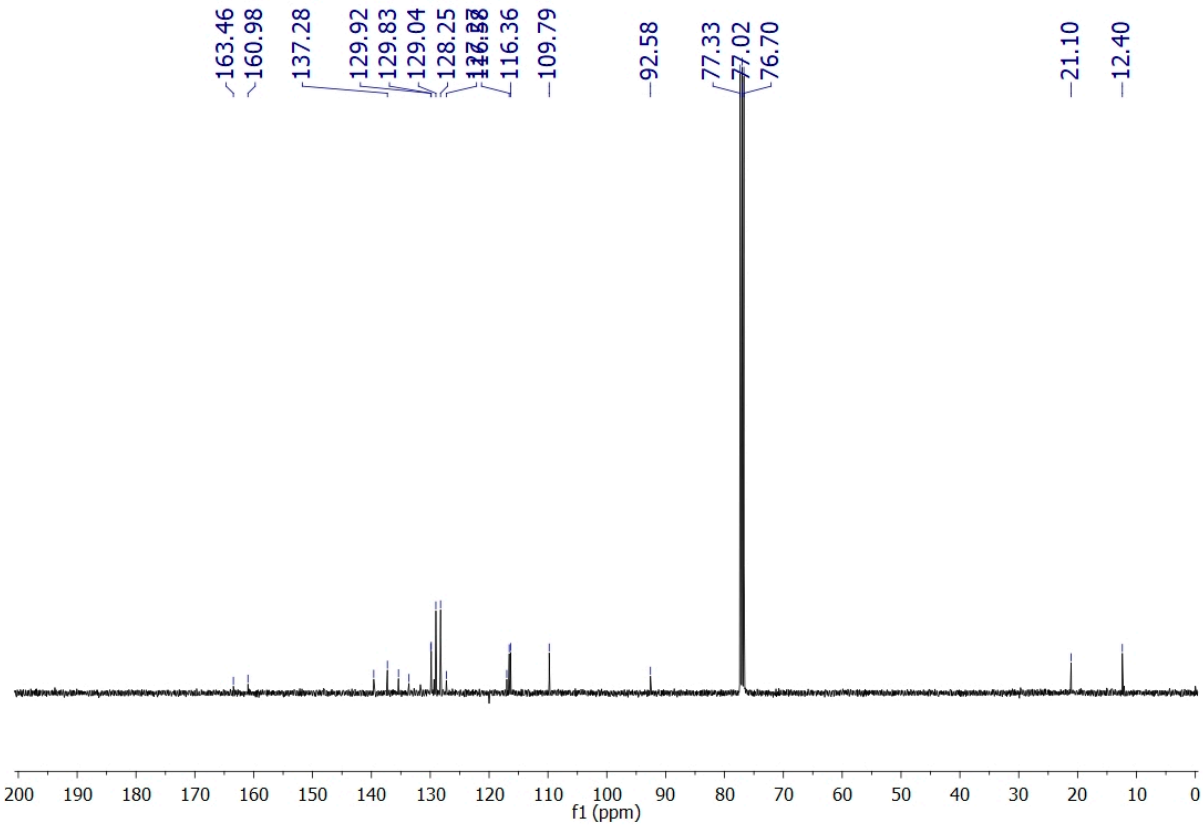
1,5-Bis(4-chlorophenyl)-2-methyl-1*H*-pyrrole-3-carbonitrile **15**





1-(4-Fluorophenyl)-2-methyl-5-(p-tolyl)-1*H*-pyrrole-3-carbonitrile **16**

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160.98
137.28
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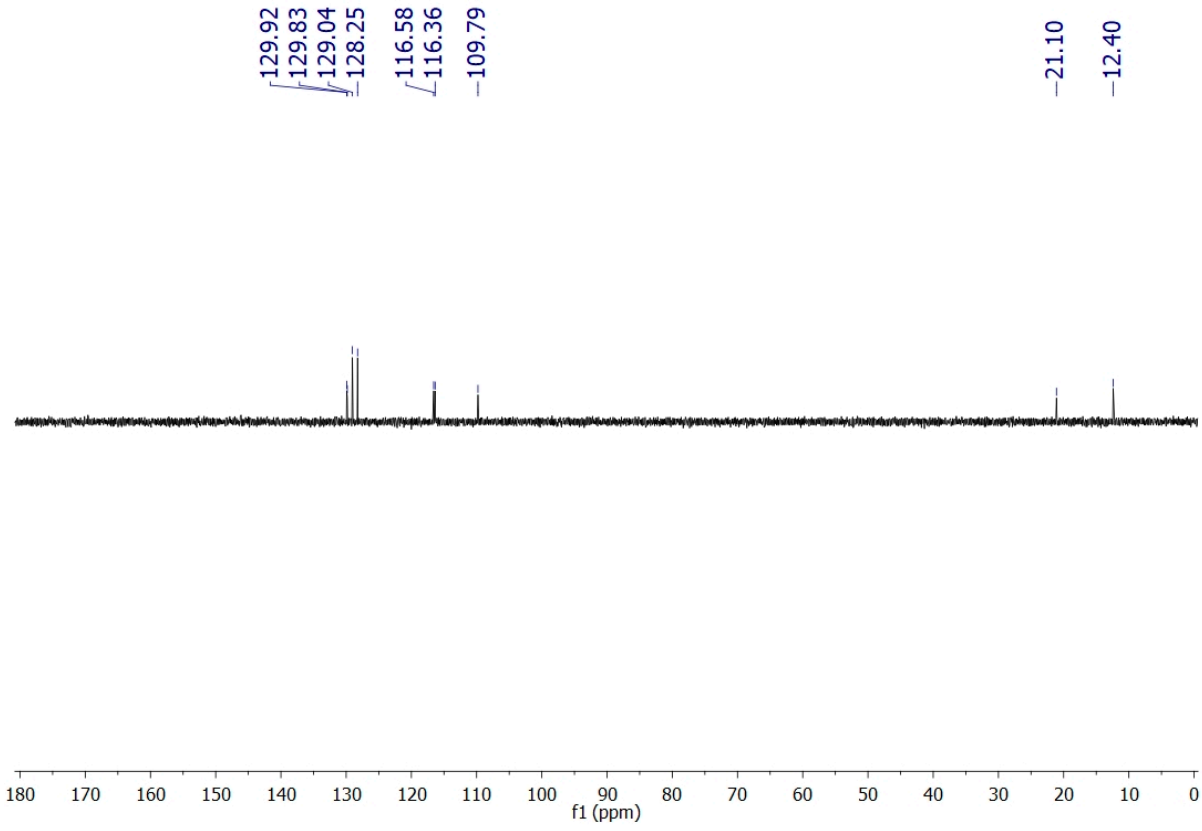
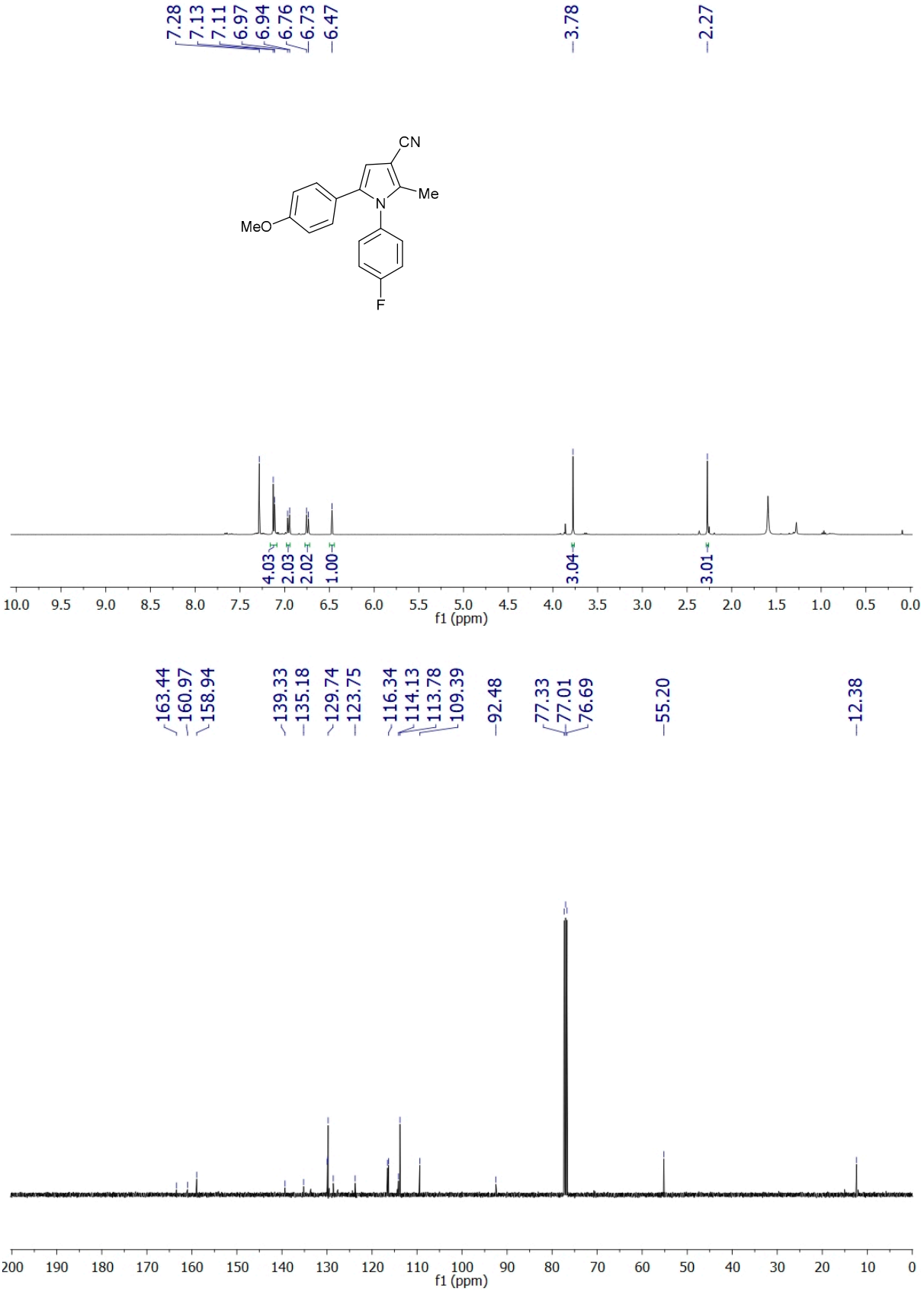
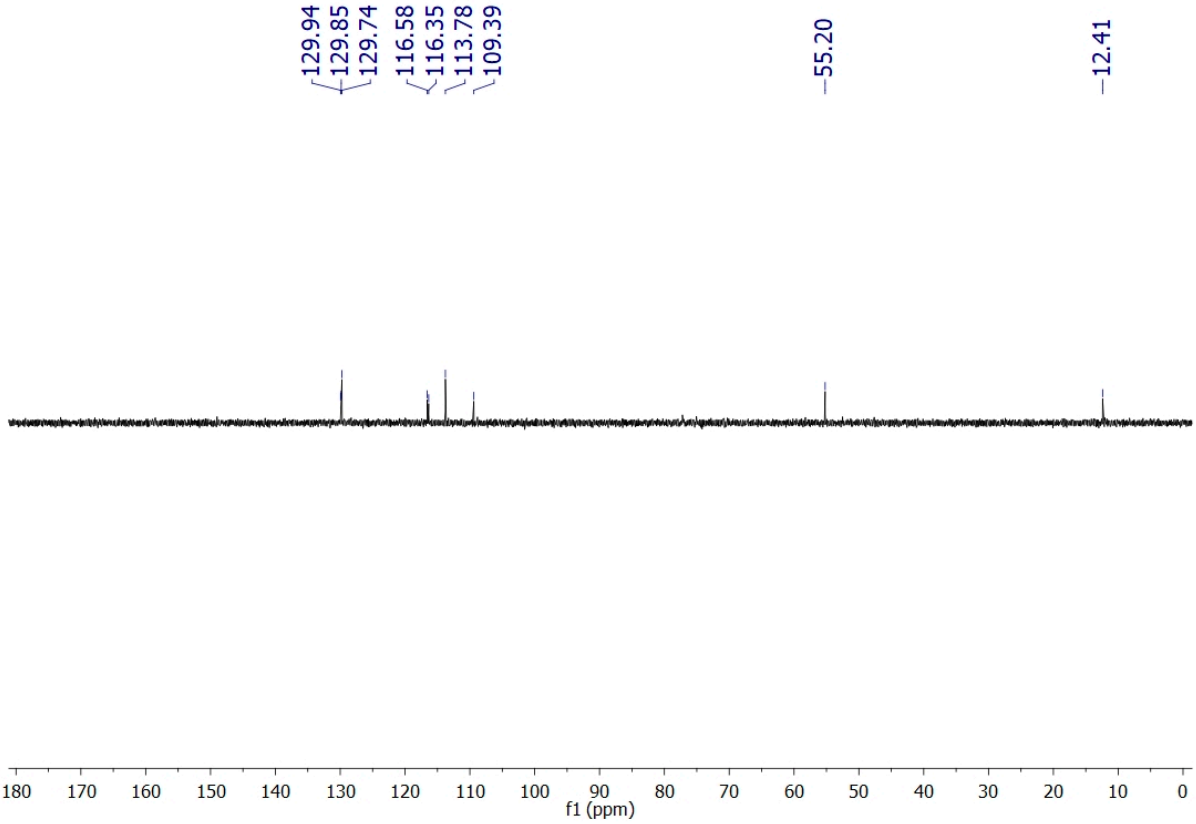
129.83
129.04
128.25
116.36
109.79
92.58
77.33
77.02
76.70
21.10
12.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

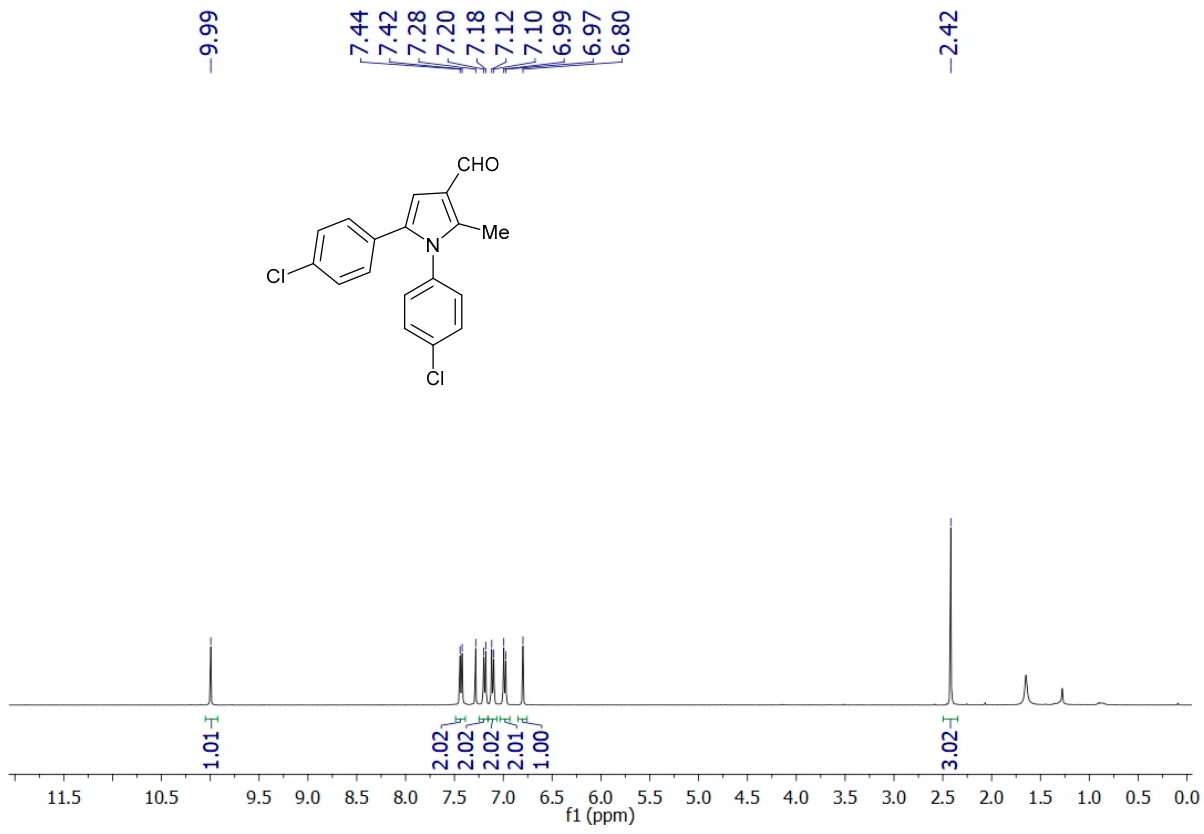

129.92
129.83
129.04
128.25
116.58
116.36
109.79
21.10
12.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

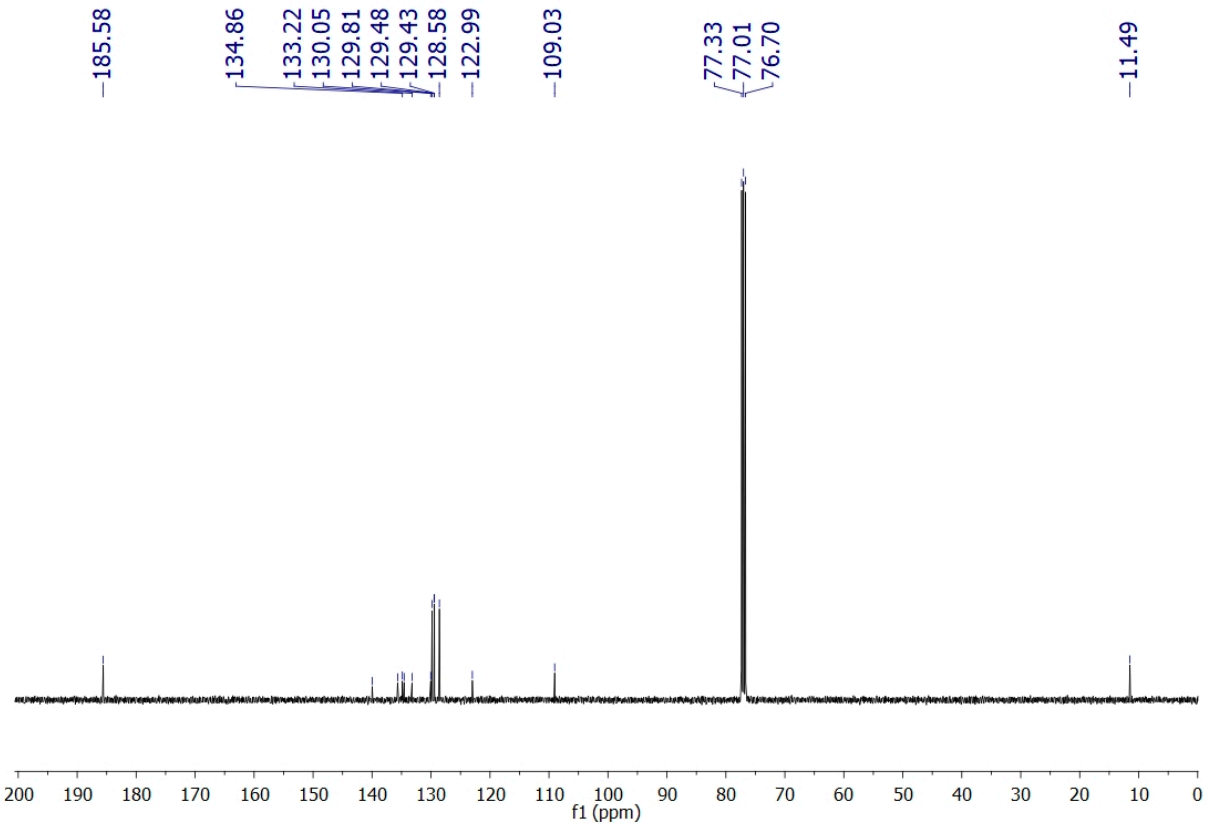
1-(4-Fluorophenyl)-5-(4-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carbonitrile **17**

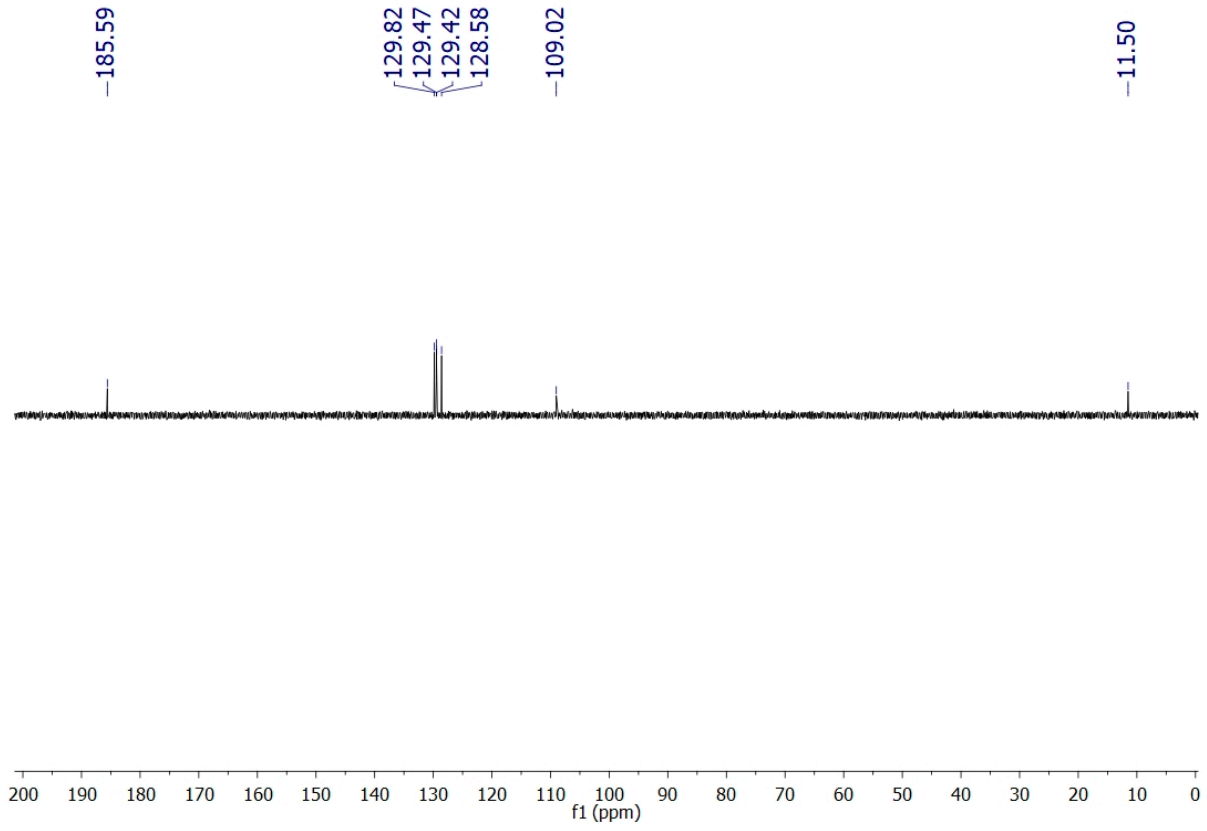




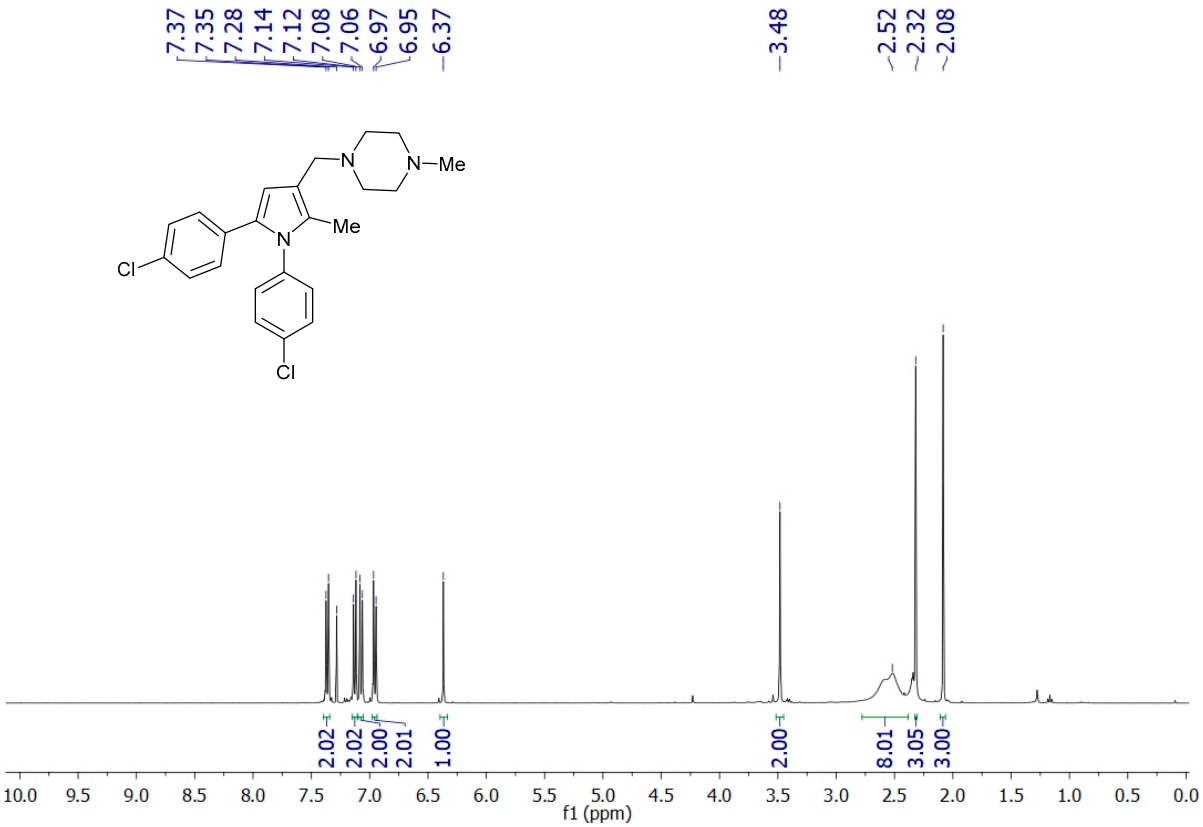
1,5-Bis(4-chlorophenyl)-2-methyl-1H-pyrrole-3-carbaldehyde **18**

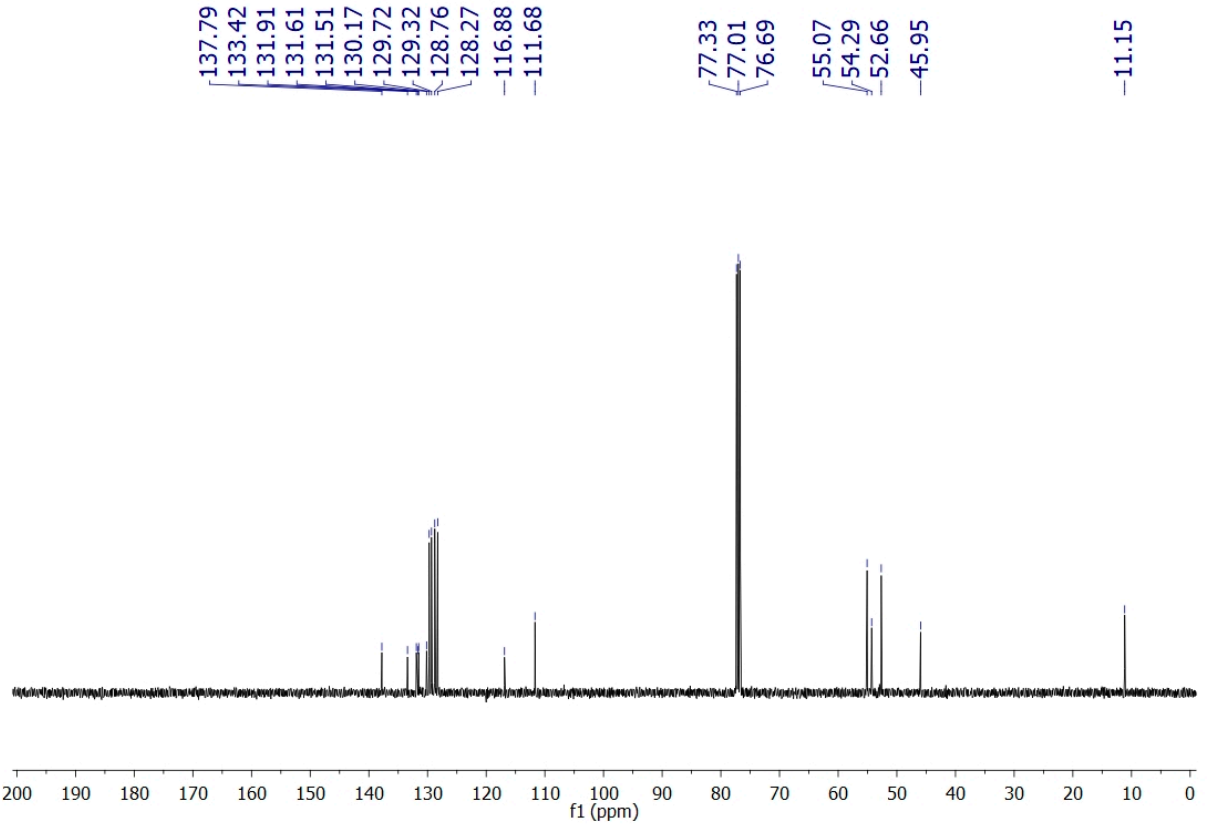


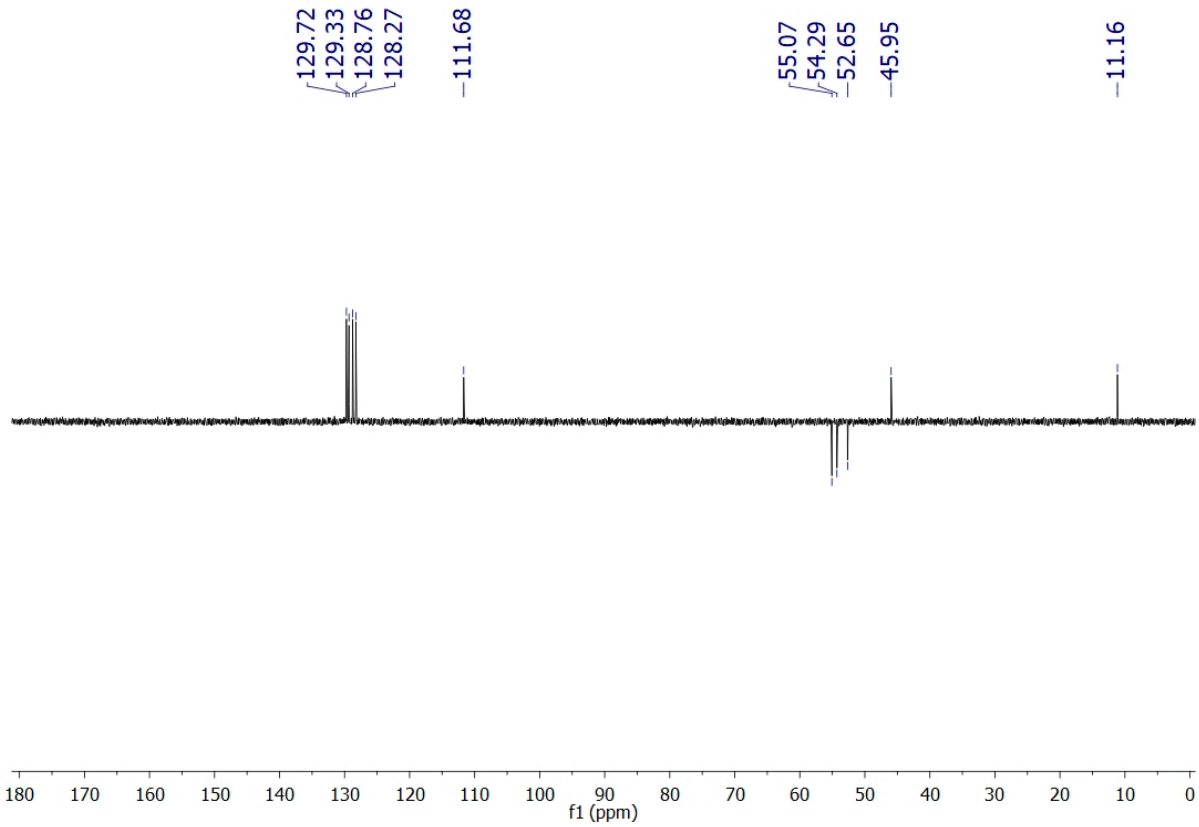

185.58
134.86
133.22
130.05
129.81
129.48
129.43
128.58
122.99
109.03
77.33
77.01
76.70
11.49
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


185.59
129.82
129.47
129.42
128.58
109.02
11.50
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

1-((1,5-Bis(4-chlorophenyl)-2-methyl-1*H*-pyrrol-3-yl)methyl)-4-methylpiperazine **2a**







2. Single-crystal XRD of BM212 (product 2a)

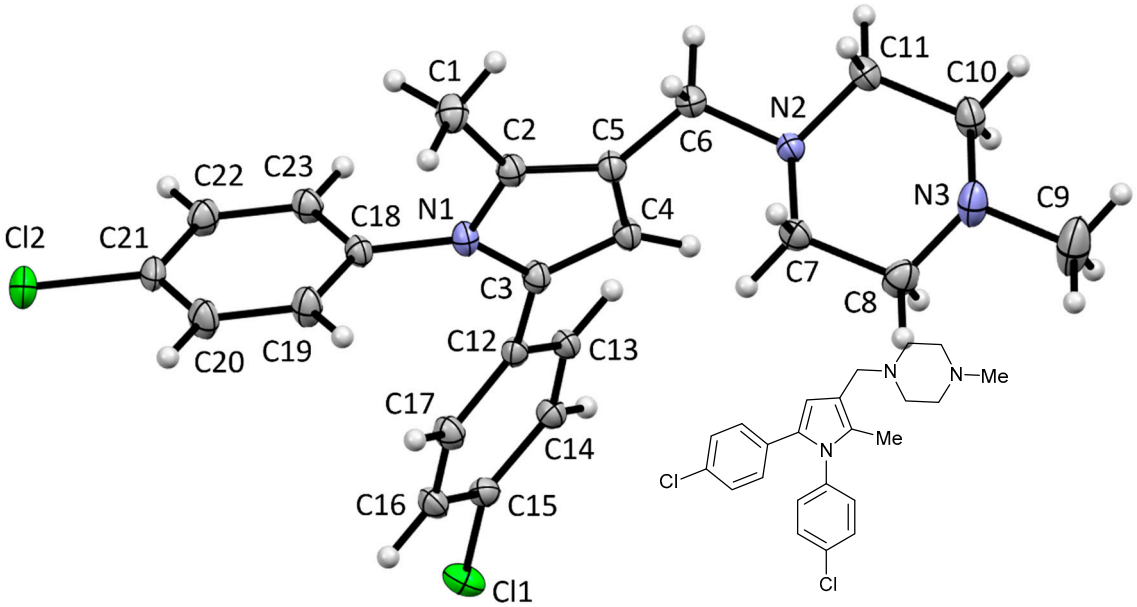


Figure S1. X-ray single crystal structure of BM212 **2a** (CCDC 2191163) (displacement ellipsoids are drawn at the 50% probability level).

Table S1. Crystal data and structure refinement for product **2a** (CCDC 2191163).

Empirical formula	$C_{23}H_{25}Cl_2N_3$
Formula weight	414.36
Temperature	100(2) K
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.1454(10) Å a= 100.119(4)°. b = 11.1138(12) Å b= 100.255(4)°. c = 11.2090(12) Å g = 106.088(4)°.
Volume	1046.2(5) $Å^3$
Z	2
Density (calculated)	1.315 Mg/m^3
F(000)	436
Reflections collected	26513
Independent reflections	8999 [R(int) = 0.0570]
Max. and min. transmission	0.9150 and 0.9030
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1200
R indices (all data)	R1 = 0.0892, wR2 = 0.1380