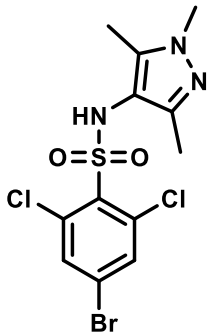
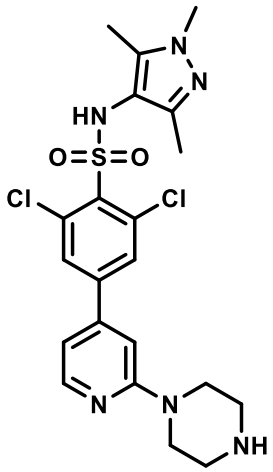


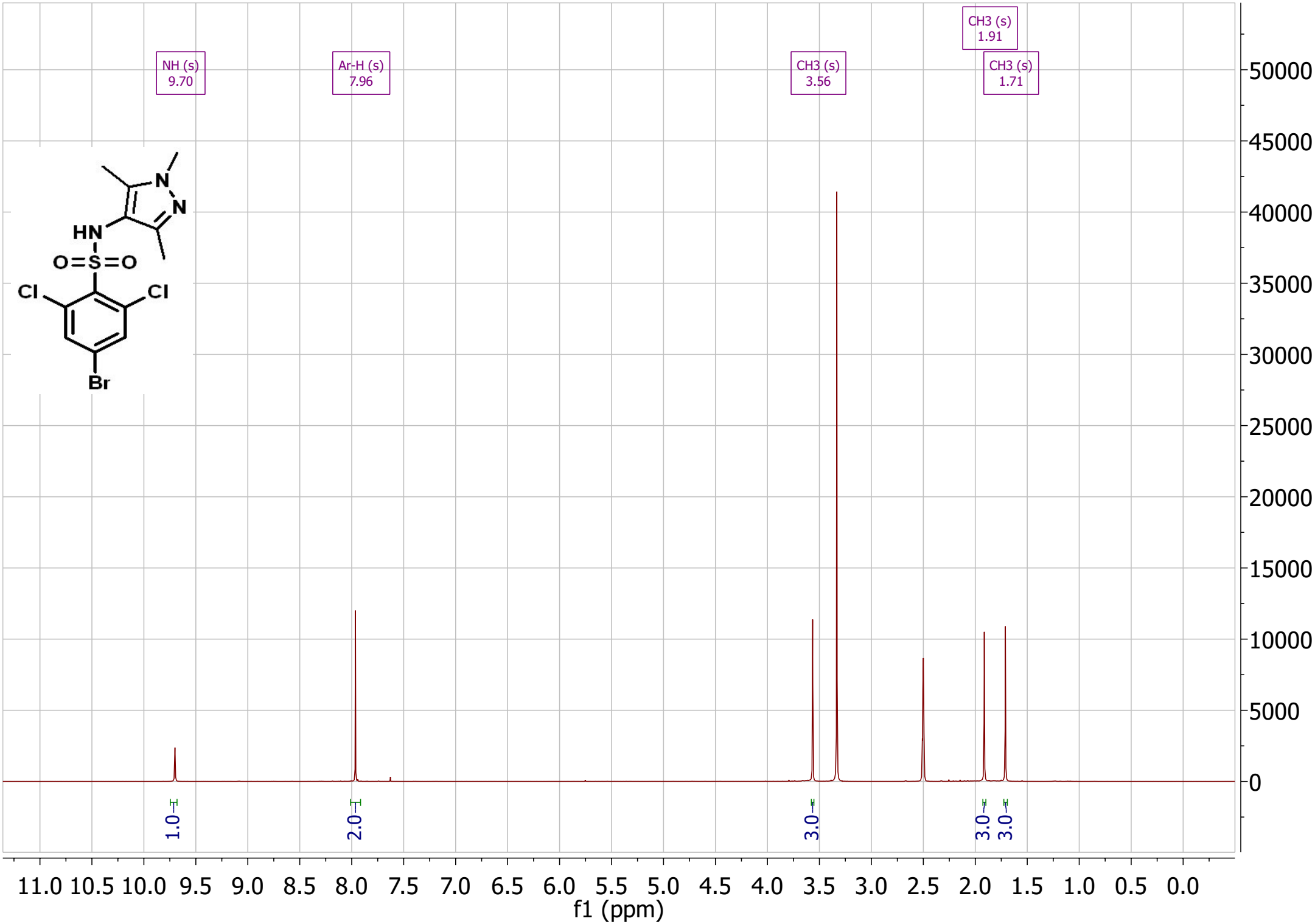
4-Bromo-2,6-dichloro-*N*-(1,3,5-trimethyl-1*H*-pyrazol-4-yl)benzenesulfonamide was synthesized according to literature [1]. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.70 (s, 1H), 7.96 (s, 2H), 3.56 (s, 3H), 1.91 (s, 3H), 1.71 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 143.8, 137.2, 135.4, 135.2, 133.8, 125.9, 111.6, 36.2, 10.4, 8.5.

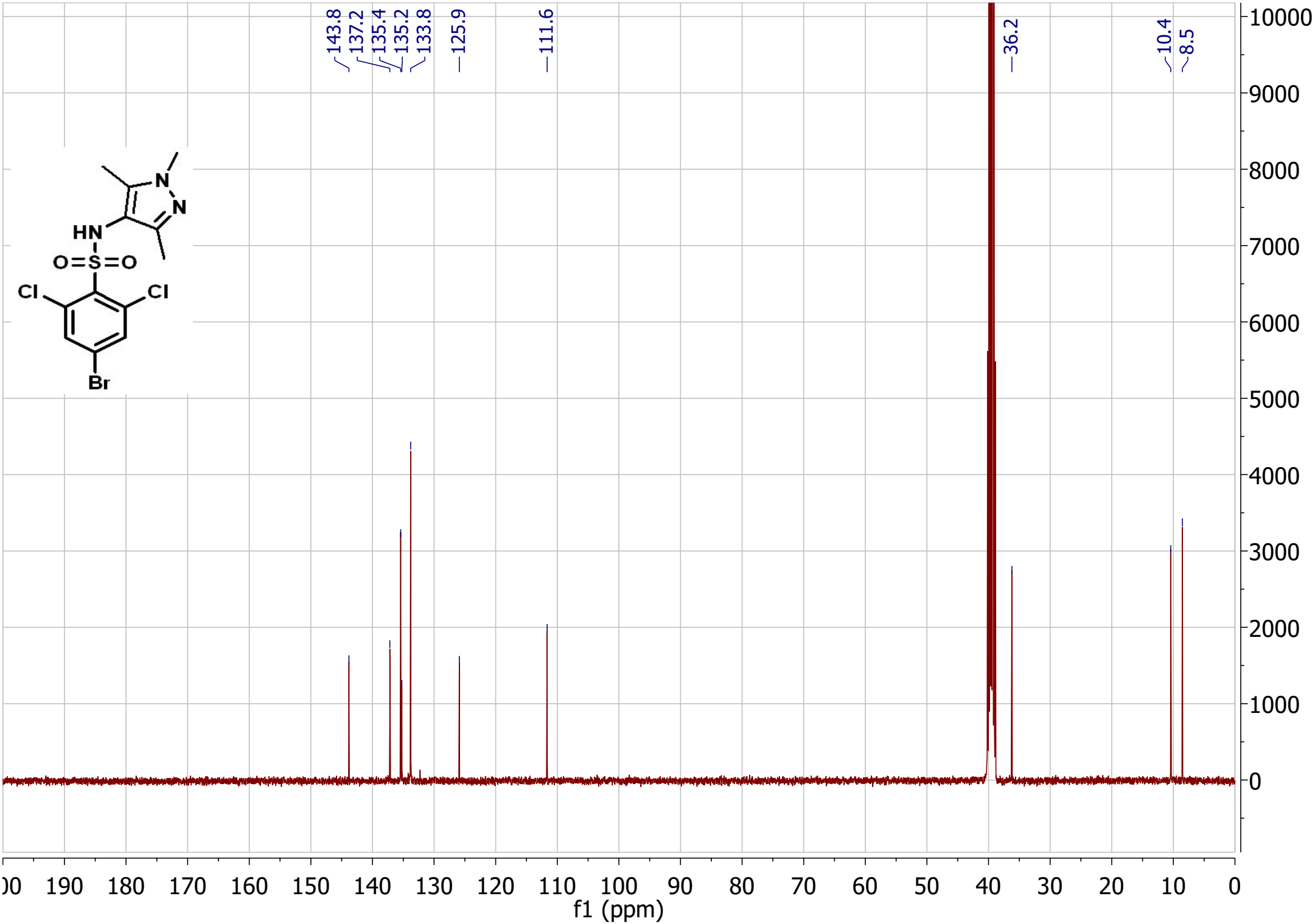


2,6-Dichloro-4-(2-(piperazin-1-yl)pyridin-4-yl)-*N*-(1,3,5-trimethyl-1*H*-pyrazol-4-yl)benzenesulfonamide (DDD85646) was synthesized according to literature [2]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 5.2 Hz, 1H), 7.64 (s, 2H), 6.75 (d, *J* = 5.1 Hz, 1H), 6.70 (s, 1H), 3.66 (s, 3H), 3.63 – 3.57 (m, 4H), 3.04 – 2.99 (m, 4H), 2.16 (s, 3H), 1.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2, 149.1, 145.3, 144.8, 144.2, 138.8, 135.9, 135.6, 129.5, 111.8, 111.0, 104.5, 46.1, 45.7, 36.6, 10.6, 9.4.

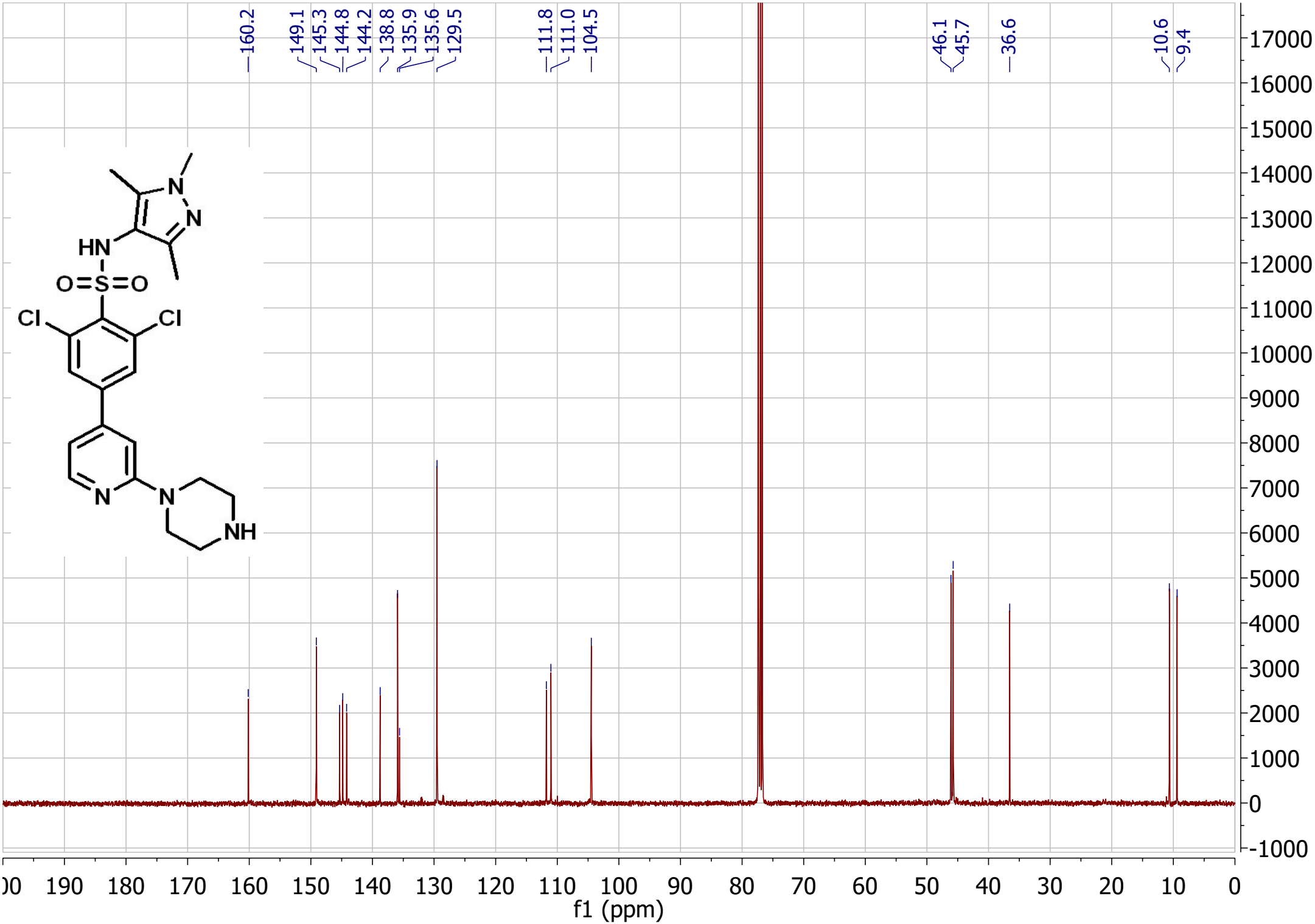
1. Frearson JA, Brand S, McElroy SP, Cleghorn LA, Smid O, Stojanovski L, et al. N-myristoyltransferase inhibitors as new leads to treat sleeping sickness. Nature. 2010;464(7289):728-32. Epub 2010/04/03. doi: 10.1038/nature08893. PubMed PMID: 20360736; PubMed Central PMCID: PMC2917743.

2. Brand S, Cleghorn LA, McElroy SP, Robinson DA, Smith VC, Hallyburton I, et al. Discovery of a novel class of orally active trypanocidal N-myristoyltransferase inhibitors. J Med Chem. 2012;55(1):140-52. doi: 10.1021/jm201091t. PubMed PMID: 22148754; PubMed Central PMCID: PMCPMC3256935.


NH (s)
9.70
Ar-H (s)
7.96
CH3 (s)
3.56
CH3 (s)
1.91
CH3 (s)
1.71
1.0
2.0
3.0
3.0
3.0
HN
N
N
O=S=O
Cl
Cl
Br
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.8
137.2
135.4
135.2
133.8
125.9
111.6
36.2
10.4
8.5
N
N
HN
O=S=O
Cl
Cl
Br
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Ar-H (d)
8.27
J(5.2)
Ar-H (s)
7.64
Ar-H (d)
6.75
J(5.1)
Ar-H (s)
6.70
CH3 (s)
3.66
CH2 (m)
3.60
CH2 (m)
3.02
CH3 (s)
2.16
CH3 (s)
1.76
HN
O=S=O
Cl
Cl
N
N
N
N
NH
1.0
2.0
1.0
1.0
3.0
3.8
3.6
3.0
3.0
f1 (ppm)


160.2
149.1
145.3
144.8
144.2
138.8
135.9
135.6
129.5
111.8
111.0
104.5
46.1
45.7
36.6
10.6
9.4
HN
O=S=O
Cl
Cl
N
N
N
N
NH
f1 (ppm)