Supporting Information

Synthesis and properties of 5,6-dihydro-dipyrrolo[1,2-*d*;1′,2′-*g*][1,4]diazepin-11-one.

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1,2-Di(pyrrol-1-yl)ethane 4[1]

Using the method of ref. 3, pyrrole (0.90 cm^3, 13.0 mmol) was added to a stirred suspension of powdered potassium hydroxide (2.90 g, 51.7 mmol, 3.98 equiv.) in DMSO (40 cm^3) and the mixture was stirred at room temperature for 3 h. The solution was then heated to 65 ºC and ethane-1,2-ditosylate (7.20 g, 19.5 mmol, 1.50 equiv.) added in 6 aliquots over the course of 60 min. The mixture was kept at 65 ºC for a further 5 h. Workup and purification by Kugelrohr distillation [50-70 ºC (1.5 Torr)] yielded 1,2-di(pyrrol-1-yl)ethane **4** as an off white solid (0.56 g, 54%) mp 107-109 ºC (from ether); (lit.,[1] 107-108 ºC) (Found: C, 74.95; H, 7.75; N, 17.45. $C_{10}H_{12}N_2$ requires C, 74.95; H, 7.55; N, 17.5%); δ_H 6.46-6.45 (4H, m), 6.14-6.12 (4H, m) and 4.18 (4H, s); δ_C 120.41 (4 CH), 108.56 (4 CH) and 50.82 (2 CH_2); *m/z* 160 (M^+, 8%), 80 (86), 53 (100) and 39 (93).

1,2-Di(pyrrol-1-yl)methane 5[1]

Pyrrole (9.00 cm^3, 130 mmol) was added to a stirred suspension of powdered potassium hydroxide (24.02 g, 0.43 mol, 3.31 equiv.) in DMSO (200 cm^3) at room temperature. After 1 h, the mixture was heated to 40 ºC and DCM (6.32 cm^3, 98.6 mmol, 0.76 equiv.) was added slowly. The solution was heated at 40 ºC for a further 4 h. Once cool, ether (100 cm^3) and water (200 cm^3) were added and the layers separated. The aqueous layer was extracted with ether (4 × 50 cm^3), the combined organic extracts were washed with water (2 × 40 cm^3), brine (2 × 40 cm^3), dried ($MgSO_4$) and the solvent removed under reduced pressure to afford a pale yellow solid. Recrystallisation from chloroform gave 1,2-di(pyrrol-1-yl)methane **5** (6.85 g, 72%) mp 99-101 ºC (from chloroform); (lit.,[1] 105 ºC) (Found: C, 73.8; H, 6.9; N, 19.15. $C_9H_{10}N_2$ requires C, 73.95; H, 6.9; N, 19.15%); δ_H 6.77 (4H, t, *J* 2.1), 6.22 (4H, t, *J* 2.1) and 5.81 (2H, s, CH_2); δ_C 119.99 (4 × CH), 109.51 (4 × CH) and 61.56 (CH_2); *m/z* 146 (M^+, 35%), 80 (100), 53 (61) and 39 (43).

Table 1. Crystal data and structure refinement for 2 (HM7003).

Contact	Anna Collins, anna.collins@ed.ac.uk
A. CRYSTAL DATA	
Empirical formula	C11 H12 N2 O2 C11 H10 N2 O1, (H2 O)
Formula weight	204.23
Wavelength	0.71073 A
Temperature	150 K
Crystal system	Orthorhombic
Space group	P 21 21 21
Unit cell dimensions	a = 4.5748(3) A alpha = 90 deg. b = 13.0074(9) A beta = 90 deg. c = 17.0717(12) A gamma = 90 deg.
Volume	1015.87(12) A^3
Number of reflections for cell	2777 (3 < theta < 31 deg.)
Z	4
Density (calculated)	1.335 Mg/m^3
Absorption coefficient	0.094 mm^-1
F(000)	432
B. DATA COLLECTION	
Crystal description	pale yellow block
Crystal size	0.32 x 0.21 x 0.17 mm
Instrument	Area
Theta range for data collection	1.968 to 30.521 deg.
Index ranges	-6<=h<=6, -15<=k<=17, -23<=l<=24
Reflections collected	7851
Independent reflections	1750 [R(int) = 0.043]
Scan type	\w
Absorption correction	Semi-empirical from equivalents (Tmin= 0.81, Tmax=0.98)
C. SOLUTION AND REFINEMENT.	
Solution	direct (SIR92 (Altomare et al., 1994))
Refinement type	Full-matrix least-squares on F^2
Program used for refinement	CRYSTALS
Hydrogen atom placement	geom
Hydrogen atom treatment	constr
Data	1742
Restraints	0
Parameters	136
Goodness-of-fit on F^2	1.0260
Conventional R [F>4sigma(F)]	R1 = 0.0703 [1426 data]
Rw	0.1841
Final maximum delta/sigma	0.000180

Weighting scheme	Sheldrick Weights
Largest diff. peak and hole	0.77 and -0.34 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2 (hm7003). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5851(9)	6862(3)	8631(2)	33
C(2)	6116(10)	6597(3)	9424(2)	39
C(3)	4374(9)	5756(3)	9550(2)	34
N(4)	3045(7)	5489(2)	8872(2)	27
C(5)	1020(9)	4627(3)	8811(2)	30
C(6)	1573(9)	3999(2)	8078(2)	30
N(7)	320(7)	4506(2)	7393(2)	28
C(8)	-1640(9)	4059(3)	6909(2)	34
C(9)	-2389(10)	4751(3)	6331(2)	39
C(10)	-784(9)	5635(3)	6464(2)	35
C(11)	2827(8)	6236(2)	7488(2)	26
C(12)	906(8)	5488(3)	7132(2)	27
C(13)	3902(8)	6171(2)	8288(2)	26
O(1)	3547(7)	7013(2)	7101(1)	36
O(15)	751(10)	2385(5)	514(2)	136

Table 3. Bond lengths [Å] and angles [deg] for 2 (hm7003).

C(1)-C(2)	1.401(5)
C(1)-C(13)	1.395(5)
C(1)-H(11)	0.932
C(2)-C(3)	1.370(6)
C(2)-H(21)	0.942
C(3)-N(4)	1.354(4)
C(3)-H(31)	0.939
N(4)-C(5)	1.459(4)
N(4)-C(13)	1.390(4)
C(5)-C(6)	1.516(5)
C(5)-H(51)	0.967
C(5)-H(52)	0.970
C(6)-N(7)	1.460(4)
C(6)-H(61)	0.975
C(6)-H(62)	0.973
N(7)-C(8)	1.351(5)
N(7)-C(12)	1.379(4)
C(8)-C(9)	1.379(5)
C(8)-H(81)	0.948
C(9)-C(10)	1.383(5)
C(9)-H(91)	0.948
C(10)-C(12)	1.391(5)
C(10)-H(101)	0.936
C(11)-C(12)	1.445(5)
C(11)-C(13)	1.455(4)
C(11)-O(1)	1.251(4)
O(15)-H(151)	0.820
O(15)-H(152)	0.820
C(2)-C(1)-C(13)	107.6(3)
C(2)-C(1)-H(11)	127.5
C(13)-C(1)-H(11)	124.9
C(1)-C(2)-C(3)	107.3(3)
C(1)-C(2)-H(21)	126.0
C(3)-C(2)-H(21)	126.6
C(2)-C(3)-N(4)	109.4(3)
C(2)-C(3)-H(31)	127.8
N(4)-C(3)-H(31)	122.9
C(3)-N(4)-C(5)	122.9(3)
C(3)-N(4)-C(13)	108.8(3)
C(5)-N(4)-C(13)	128.2(3)
N(4)-C(5)-C(6)	111.5(3)
N(4)-C(5)-H(51)	107.1
C(6)-C(5)-H(51)	110.2
N(4)-C(5)-H(52)	109.5
C(6)-C(5)-H(52)	108.2

H(51)-C(5)-H(52)	110.4
C(5)-C(6)-N(7)	110.6(3)
C(5)-C(6)-H(61)	109.2
N(7)-C(6)-H(61)	109.1
C(5)-C(6)-H(62)	110.4
N(7)-C(6)-H(62)	107.0
H(61)-C(6)-H(62)	110.5
C(6)-N(7)-C(8)	123.7(3)
C(6)-N(7)-C(12)	127.0(3)
C(8)-N(7)-C(12)	109.3(3)
N(7)-C(8)-C(9)	108.7(3)
N(7)-C(8)-H(81)	125.1
C(9)-C(8)-H(81)	126.2
C(8)-C(9)-C(10)	107.1(3)
C(8)-C(9)-H(91)	126.9
C(10)-C(9)-H(91)	126.0
C(9)-C(10)-C(12)	108.4(3)
C(9)-C(10)-H(101)	126.5
C(12)-C(10)-H(101)	125.1
C(12)-C(11)-C(13)	124.1(3)
C(12)-C(11)-O(1)	118.9(3)
C(13)-C(11)-O(1)	116.9(3)
C(11)-C(12)-C(10)	126.2(3)
C(11)-C(12)-N(7)	127.3(3)
C(10)-C(12)-N(7)	106.5(3)
C(11)-C(13)-C(1)	125.0(3)
C(11)-C(13)-N(4)	128.0(3)
C(1)-C(13)-N(4)	106.9(3)
H(151)-O(15)-H(152)	130.4

Symmetry transformations used to generate equivalent atoms:

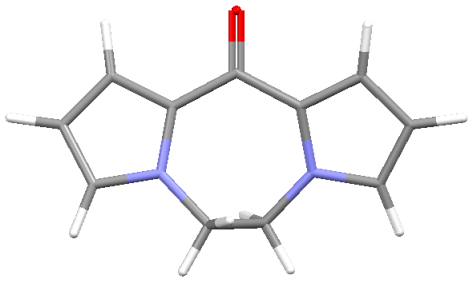
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 2 (hm7003). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	29(2)	25(2)	45(2)	-2(1)	-6(2)	0(2)
C(2)	36(2)	41(2)	41(2)	-15(2)	-10(2)	6(2)
C(3)	34(2)	40(2)	26(2)	-4(1)	-3(2)	9(2)
N(4)	24(1)	30(1)	26(1)	-1(1)	0(1)	7(1)
C(5)	29(2)	31(2)	31(2)	3(1)	4(2)	1(2)
C(6)	29(2)	24(1)	36(2)	1(1)	2(2)	1(1)
N(7)	26(2)	26(1)	30(1)	-3(1)	5(1)	-2(1)
C(8)	30(2)	36(2)	35(2)	-13(2)	3(2)	-3(2)
C(9)	29(2)	59(2)	30(2)	-10(2)	1(2)	-6(2)
C(10)	32(2)	47(2)	25(1)	-1(2)	1(2)	5(2)
C(11)	25(2)	24(1)	29(1)	0(1)	4(1)	4(1)
C(12)	29(2)	29(2)	23(1)	-3(1)	5(1)	5(2)
C(13)	26(2)	23(1)	29(1)	1(1)	1(1)	3(1)
O(1)	44(2)	29(1)	34(1)	4(1)	3(1)	-4(1)
O(15)	72(3)	289(8)	48(2)	22(3)	-27(2)	-99(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2 (hm7003).

	x	y	z	U(eq)
H(11)	6774	7400	8369	39
H(21)	7292	6933	9797	47
H(31)	4121	5389	10018	41
H(51)	1299	4206	9272	36
H(52)	-970	4883	8790	36
H(61)	3674	3921	8002	35
H(62)	641	3328	8120	36
H(81)	-2410	3387	6971	42
H(91)	-3771	4652	5925	46
H(101)	-840	6240	6167	42
H(151)	967	2559	972	151
H(152)	-657	2449	221	151

Table 6. Gas-phase structure of 2 calculated at MP2 level using the 6-31G basis set.[2]



C	-2.557653	1.212464	-0.229177
C	-1.307314	0.593108	-0.011387
N	-1.559346	-0.772832	0.220742
C	-2.936377	-1.002744	0.151733
C	-3.570299	0.215824	-0.126766
C	0.000018	1.283936	0.000255
C	-0.570778	-1.825778	0.514469
O	-0.000024	2.563952	0.000821
C	1.307379	0.593170	0.010902
C	2.557786	1.212505	0.228403
C	3.570356	0.215776	0.126183
C	2.936312	-1.002862	-0.151736
N	1.559281	-0.772899	-0.220618
C	0.570684	-1.825921	-0.514000
H	-2.683608	2.269530	-0.436673
H	-3.340043	-1.998118	0.307403
H	-4.638678	0.358432	-0.250712
H	-1.108789	-2.782989	0.474688
H	-0.159705	-1.700705	1.526987
H	2.683827	2.269646	0.435464
H	4.638775	0.358390	0.249765
H	3.339901	-1.998308	-0.307144
H	0.159594	-1.701138	-1.526546
H	1.108699	-2.783118	-0.473954

Table 7. Crystal data and structure refinement for 3 (hm7004).

Contact	Fraser J. White, f.j.white@sms.ed.ac.uk
A. CRYSTAL DATA	
Empirical formula	C10 H8 N2 O C10 H8 N2 O
Formula weight	172.18
Wavelength	0.71073 A
Temperature	150(2) K
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 7.6509(2) A alpha = 102.228(2) deg. b = 9.1569(3) A beta = 93.332(2) deg. c = 12.0975(4) A gamma = 99.815(2) deg.
Volume	812.26(4) A^3
Number of reflections for cell	? (? < theta < ? deg.)
Z	4
Density (calculated)	1.408 Mg/m^3
Absorption coefficient	0.094 mm^-1
F(000)	360
B. DATA COLLECTION	
Crystal description	orange block
Crystal size	0.28 x 0.25 x 0.13 mm
Instrument	Bruker Smart Apex CCD
Theta range for data collection	1.73 to 30.53 deg.
Index ranges	-10<=h<=10, -12<=k<=12, -16<=l<=17
Reflections collected	11866
Independent reflections	4583 [R(int) = 0.0416]
Scan type	Omega Scans
Absorption correction	Semi-empirical from equivalents (Tmin= 0.8167, Tmax=0.9849)
C. SOLUTION AND REFINEMENT.	
Solution	direct (Shelxs Sheldrick)
Refinement type	Full-matrix least-squares on F^2
Program used for refinement	SHELXL-97
Hydrogen atom placement	geom
Hydrogen atom treatment	constr
Data / restraints / parameters	4583/ 0/ 235
Goodness-of-fit on F^2	1.026
Conventional R [F>4sigma(F)]	R1 = 0.0597 [3122 data]
Rw	0.1396
Final maximum delta/sigma	0.000
Weighting scheme	

calc w=1/[\s^2^(Fo^2^)+(0.0520P)^2^+0.2206P] where P=(Fo^2^+2Fc^2^)/3
Largest diff. peak and hole 0.281 and -0.220 e.A^-3

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 3 (hm7004). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1A)	5609(3)	2026(2)	11543(2)	33(1)
C(2A)	6300(3)	2710(2)	12669(2)	39(1)
C(3A)	7261(3)	4124(2)	12675(2)	35(1)
N(4A)	7201(2)	4316(2)	11596(1)	27(1)
C(5A)	7899(3)	5717(2)	11266(2)	31(1)
N(6A)	7883(2)	5430(2)	10043(1)	27(1)
C(7A)	8722(3)	6414(2)	9461(2)	35(1)
C(8A)	8223(3)	5838(2)	8323(2)	38(1)
C(9A)	7039(3)	4460(2)	8204(2)	33(1)
C(10A)	6818(2)	4218(2)	9281(1)	25(1)
O(11A)	4843(2)	1875(1)	9032(1)	33(1)
C(11A)	5851(2)	2955(2)	9679(1)	25(1)
C(12A)	6162(2)	3040(2)	10885(1)	26(1)
C(1B)	1940(3)	9455(2)	2298(2)	33(1)
C(2B)	983(3)	10018(2)	1512(2)	36(1)
C(3B)	-741(3)	9934(2)	1806(2)	34(1)
N(4B)	-863(2)	9322(2)	2731(1)	28(1)
C(5B)	-2384(2)	9215(2)	3392(1)	31(1)
N(6B)	-2199(2)	8181(2)	4131(1)	30(1)
C(7B)	-3501(3)	7578(2)	4702(2)	39(1)
C(8B)	-2760(3)	6844(3)	5437(2)	41(1)
C(9B)	-925(3)	7032(2)	5322(2)	35(1)
C(10B)	-586(2)	7874(2)	4517(1)	29(1)
O(11B)	2486(2)	8088(2)	4337(1)	37(1)
C(11B)	1023(2)	8325(2)	4001(1)	29(1)
C(12B)	791(2)	9037(2)	3059(1)	27(1)

Table 9. Bond lengths [Å] and angles [deg] for 3 (hm7004).

C(1A)-C(12A)	1.376(2)
C(1A)-C(2A)	1.403(3)
C(1A)-H(1A)	0.9500
C(2A)-C(3A)	1.374(3)
C(2A)-H(2A)	0.9500
C(3A)-N(4A)	1.351(2)
C(3A)-H(3A)	0.9500
N(4A)-C(12A)	1.384(2)
N(4A)-C(5A)	1.449(2)
C(5A)-N(6A)	1.445(2)
C(5A)-H(5A1)	0.9900
C(5A)-H(5A2)	0.9900
N(6A)-C(7A)	1.358(2)
N(6A)-C(10A)	1.385(2)
C(7A)-C(8A)	1.371(3)
C(7A)-H(7A)	0.9500
C(8A)-C(9A)	1.397(3)
C(8A)-H(8A)	0.9500
C(9A)-C(10A)	1.382(2)
C(9A)-H(9A)	0.9500
C(10A)-C(11A)	1.450(2)
O(11A)-C(11A)	1.236(2)
C(11A)-C(12A)	1.447(2)
C(1B)-C(12B)	1.378(3)
C(1B)-C(2B)	1.400(3)
C(1B)-H(1B)	0.9500
C(2B)-C(3B)	1.380(3)
C(2B)-H(2B)	0.9500
C(3B)-N(4B)	1.355(2)
C(3B)-H(3B)	0.9500
N(4B)-C(12B)	1.387(2)
N(4B)-C(5B)	1.451(2)
C(5B)-N(6B)	1.451(2)
C(5B)-H(5B1)	0.9900
C(5B)-H(5B2)	0.9900
N(6B)-C(7B)	1.352(2)
N(6B)-C(10B)	1.388(2)
C(7B)-C(8B)	1.374(3)
C(7B)-H(7B)	0.9500
C(8B)-C(9B)	1.404(3)
C(8B)-H(8B)	0.9500
C(9B)-C(10B)	1.375(3)
C(9B)-H(9B)	0.9500
C(10B)-C(11B)	1.449(3)

O(11B)-C(11B)	1.238(2)
C(11B)-C(12B)	1.444(3)

C(12A)-C(1A)-C(2A)	107.48(17)
C(12A)-C(1A)-H(1A)	126.3
C(2A)-C(1A)-H(1A)	126.3
C(3A)-C(2A)-C(1A)	107.54(17)
C(3A)-C(2A)-H(2A)	126.2
C(1A)-C(2A)-H(2A)	126.2
N(4A)-C(3A)-C(2A)	108.37(17)
N(4A)-C(3A)-H(3A)	125.8
C(2A)-C(3A)-H(3A)	125.8
C(3A)-N(4A)-C(12A)	109.24(16)
C(3A)-N(4A)-C(5A)	125.05(15)
C(12A)-N(4A)-C(5A)	125.17(14)
N(6A)-C(5A)-N(4A)	109.52(14)
N(6A)-C(5A)-H(5A1)	109.8
N(4A)-C(5A)-H(5A1)	109.8
N(6A)-C(5A)-H(5A2)	109.8
N(4A)-C(5A)-H(5A2)	109.8
H(5A1)-C(5A)-H(5A2)	108.2
C(7A)-N(6A)-C(10A)	109.07(15)
C(7A)-N(6A)-C(5A)	125.01(15)
C(10A)-N(6A)-C(5A)	125.34(15)
N(6A)-C(7A)-C(8A)	108.34(17)
N(6A)-C(7A)-H(7A)	125.8
C(8A)-C(7A)-H(7A)	125.8
C(7A)-C(8A)-C(9A)	107.80(17)
C(7A)-C(8A)-H(8A)	126.1
C(9A)-C(8A)-H(8A)	126.1
C(10A)-C(9A)-C(8A)	107.60(17)
C(10A)-C(9A)-H(9A)	126.2
C(8A)-C(9A)-H(9A)	126.2
C(9A)-C(10A)-N(6A)	107.17(16)
C(9A)-C(10A)-C(11A)	132.38(16)
N(6A)-C(10A)-C(11A)	120.25(15)
O(11A)-C(11A)-C(12A)	122.37(16)
O(11A)-C(11A)-C(10A)	122.27(16)
C(12A)-C(11A)-C(10A)	115.36(15)
C(1A)-C(12A)-N(4A)	107.35(16)
C(1A)-C(12A)-C(11A)	131.91(17)
N(4A)-C(12A)-C(11A)	120.73(15)
C(12B)-C(1B)-C(2B)	107.72(17)
C(12B)-C(1B)-H(1B)	126.1
C(2B)-C(1B)-H(1B)	126.1
C(3B)-C(2B)-C(1B)	107.55(18)
C(3B)-C(2B)-H(2B)	126.2
C(1B)-C(2B)-H(2B)	126.2
N(4B)-C(3B)-C(2B)	108.24(17)

N(4B)-C(3B)-H(3B)	125.9
C(2B)-C(3B)-H(3B)	125.9
C(3B)-N(4B)-C(12B)	109.22(16)
C(3B)-N(4B)-C(5B)	125.56(15)
C(12B)-N(4B)-C(5B)	124.48(15)
N(6B)-C(5B)-N(4B)	109.13(14)
N(6B)-C(5B)-H(5B1)	109.9
N(4B)-C(5B)-H(5B1)	109.9
N(6B)-C(5B)-H(5B2)	109.9
N(4B)-C(5B)-H(5B2)	109.9
H(5B1)-C(5B)-H(5B2)	108.3
C(7B)-N(6B)-C(10B)	108.93(16)
C(7B)-N(6B)-C(5B)	125.61(16)
C(10B)-N(6B)-C(5B)	124.57(15)
N(6B)-C(7B)-C(8B)	108.60(17)
N(6B)-C(7B)-H(7B)	125.7
C(8B)-C(7B)-H(7B)	125.7
C(7B)-C(8B)-C(9B)	107.47(18)
C(7B)-C(8B)-H(8B)	126.3
C(9B)-C(8B)-H(8B)	126.3
C(10B)-C(9B)-C(8B)	107.52(17)
C(10B)-C(9B)-H(9B)	126.2
C(8B)-C(9B)-H(9B)	126.2
C(9B)-C(10B)-N(6B)	107.45(16)
C(9B)-C(10B)-C(11B)	131.94(17)
N(6B)-C(10B)-C(11B)	120.39(16)
O(11B)-C(11B)-C(12B)	122.68(17)
O(11B)-C(11B)-C(10B)	121.94(17)
C(12B)-C(11B)-C(10B)	115.37(16)
C(1B)-C(12B)-N(4B)	107.27(16)
C(1B)-C(12B)-C(11B)	131.76(17)
N(4B)-C(12B)-C(11B)	120.83(16)

Symmetry transformations used to generate equivalent atoms:

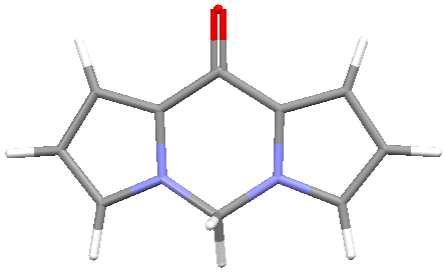
Table 10. Anisotropic displacement parameters (A^2 x 10^3) for 3 (hm7004). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1A)	29(1)	32(1)	40(1)	12(1)	10(1)	8(1)
C(2A)	43(1)	49(1)	33(1)	19(1)	12(1)	20(1)
C(3A)	41(1)	42(1)	25(1)	6(1)	2(1)	17(1)
N(4A)	28(1)	28(1)	25(1)	5(1)	-1(1)	7(1)
C(5A)	34(1)	23(1)	31(1)	3(1)	-5(1)	3(1)
N(6A)	25(1)	24(1)	31(1)	6(1)	0(1)	3(1)
C(7A)	30(1)	27(1)	49(1)	14(1)	3(1)	2(1)
C(8A)	38(1)	41(1)	41(1)	19(1)	12(1)	10(1)
C(9A)	33(1)	36(1)	30(1)	8(1)	4(1)	9(1)
C(10A)	23(1)	25(1)	27(1)	4(1)	-1(1)	5(1)
O(11A)	30(1)	29(1)	35(1)	2(1)	-3(1)	-1(1)
C(11A)	21(1)	24(1)	30(1)	3(1)	1(1)	5(1)
C(12A)	22(1)	26(1)	30(1)	6(1)	3(1)	6(1)
C(1B)	27(1)	33(1)	38(1)	5(1)	0(1)	3(1)
C(2B)	36(1)	36(1)	36(1)	11(1)	6(1)	6(1)
C(3B)	38(1)	32(1)	32(1)	7(1)	-3(1)	8(1)
N(4B)	25(1)	30(1)	28(1)	2(1)	-1(1)	7(1)
C(5B)	24(1)	41(1)	27(1)	2(1)	-2(1)	13(1)
N(6B)	23(1)	41(1)	25(1)	4(1)	-1(1)	10(1)
C(7B)	24(1)	58(1)	33(1)	6(1)	3(1)	8(1)
C(8B)	34(1)	60(1)	30(1)	13(1)	7(1)	8(1)
C(9B)	32(1)	47(1)	28(1)	8(1)	0(1)	12(1)
C(10B)	24(1)	37(1)	25(1)	1(1)	-2(1)	9(1)
O(11B)	24(1)	52(1)	34(1)	7(1)	-2(1)	13(1)
C(11B)	25(1)	32(1)	27(1)	-1(1)	-2(1)	7(1)
C(12B)	22(1)	28(1)	29(1)	1(1)	-2(1)	5(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 3 (hm7004).

	x	y	z	U(eq)
H(1A)	4890	1043	11283	39
H(2A)	6134	2275	13310	46
H(3A)	7865	4845	13325	42
H(5A1)	7162	6488	11530	37
H(5A2)	9133	6118	11623	37
H(7A)	9519	7342	9786	41
H(8A)	8613	6295	7723	45
H(9A)	6487	3808	7509	39
H(1B)	3163	9376	2304	40
H(2B)	1438	10390	889	43
H(3B)	-1680	10250	1425	41
H(5B1)	-2447	10233	3852	37
H(5B2)	-3497	8836	2877	37
H(7B)	-4722	7650	4611	46
H(8B)	-3378	6306	5933	49
H(9B)	-73	6648	5727	42

Table 12. Gas-phase structure of 3 calculated at MP2 level using the 6-31G basis set.[2]



C	-2.580250	0.932308	-0.146171
C	-1.244482	0.561749	0.091663
N	-1.190693	-0.845726	0.060745
C	-2.472823	-1.357529	-0.142483
C	-3.346570	-0.267576	-0.276612
C	-0.000037	1.349315	0.143273
C	0.000024	-1.612973	0.451039
O	-0.000036	2.621767	0.193031
C	1.244382	0.561780	0.090929
C	2.580228	0.932358	-0.146320
C	3.346614	-0.267534	-0.276496
C	2.472952	-1.357488	-0.142021
N	1.190672	-0.845718	0.060453
H	-2.934273	1.954578	-0.227559
H	-2.657339	-2.426747	-0.168203
H	-4.411297	-0.337212	-0.472946
H	-0.000064	-2.576581	-0.073861
H	0.000162	-1.785299	1.538157
H	2.934158	1.954605	-0.228444
H	4.411556	-0.337132	-0.471672
H	2.657292	-2.426707	-0.168910

Table 13. Comparison of X-Ray structures (bond lengths/Å and bond angles/°) of 2 and 3 and corresponding data from *ab initio* calculations.

2	Crystal	MP2/6-31G[a]	3	Crystal	MP2/6-31G[a]
C(1)-C(2)	1.401(5)	1.4245	C(1A)-C(12A)	1.376(2)	1.4064
C(1)-C(13)	1.395(5)	1.4122	C(1A)-(2A)	1.403(3)	1.4297
C(2)-C(3)	1.370(6)	1.4015	C(2A)-C(3A)	1.374(3)	1.4033
C(3)-N(4)	1.354(4)	1.3978	C(3A)-N(4A)	1.351(2)	1.3954
N(4)-C(5)	1.459(4)	1.4739	N(4A)-C(12A)	1.384(2)	1.4088
N(4)-C(13)	1.390(4)	1.4083	N(4A)-C(5A)	1.449(2)	1.4690
C(5)-C(6)	1.516(5)	1.5365	C(5A)-N(6A)	1.445(2)	1.4690
C(6)-N(7)	1.460(4)	1.4739	N(6A)-C(7A)	1.358(2)	1.3954
N(7)-C(8)	1.351(5)	1.3978	N(6A)-C(10A)	1.385(2)	1.4089
N(7)-C(12)	1.379(4)	1.4083	C(7A)-C(8A)	1.371(3)	1.4033
C(8)-C(9)	1.379(5)	1.4015	C(8A)-C(9A)	1.397(3)	1.4297
C(9)-C(10)	1.383(5)	1.4245	C(9A)-C(10A)	1.382(2)	1.4064
C(10)-C(12)	1.391(5)	1.4122	C(10A)-C(11A)	1.450(2)	1.4736
C(11)-C(12)	1.445(5)	1.4787	O(11A)-C(11A)	1.236(2)	1.2734
C(11)-C(13)	1.455(4)	1.4787	C(11A)-C(12A)	1.447(2)	1.4736
C(11)-O(1)	1.251(4)	1.2800			
C(2)-C(1)-C(13)	107.6(3)	108.15	C(12A)-C(1A)-C(2A)	107.48(17)	107.66
C(1)-C(2)-C(3)	107.3(3)	107.52	C(3A)-C(2A)-C(1A)	107.54(17)	108.02
C(2)-C(3)-N(4)	109.4(3)	108.20	N(4A)-C(3A)-C(2A)	108.37(17)	107.53
C(3)-N(4)-C(5)	122.9(3)	123.58	C(3A)-N(4A)-C(12A)	109.24(16)	109.54
C(3)-N(4)-C(13)	108.8(3)	109.13	C(3A)-N(4A)-C(5A)	125.05(15)	126.28
C(5)-N(4)-C(13)	128.2(3)	127.29	C(12A)-N(4A)-C(5A)	125.17(14)	123.15
N(4)-C(5)-C(6)	111.5(3)	111.41	N(6A)-C(5A)-N(4A)	109.52(14)	108.26
C(5)-C(6)-N(7)	110.6(3)	111.41	C(7A)-N(6A)-C(10A)	109.07(15)	109.54
C(6)-N(7)-C(8)	123.7(3)	123.58	C(7A)-N(6A)-C(5A)	125.01(15)	126.28
C(6)-N(7)-C(12)	127.0(3)	127.28	C(10A)-N(6A)-C(5A)	125.34(15)	123.15
C(8)-N(7)-C(12)	109.3(3)	109.13	N(6A)-C(7A)-C(8A)	108.34(17)	107.53
N(7)-C(8)-C(9)	108.7(3)	108.20	C(7A)-C(8A)-C(9A)	107.80(17)	108.02
C(8)-C(9)-C(10)	107.1(3)	107.52	C(10A)-C(9A)-C(8A)	107.60(17)	107.66
C(9)-C(10)-C(12)	108.4(3)	108.15	C(9A)-C(10A)-N(6A)	107.17(16)	107.21
C(12)-C(11)-C(13)	124.1(3)	124.30	C(9A)-C(10A)-C(11A)	132.38(16)	131.86
C(12)-C(11)-O(1)	118.9(3)	117.85	N(6A)-C(10A)-C(11A)	120.25(15)	120.16
C(13)-C(11)-O(1)	116.9(3)	117.85	O(11A)-C(11A)-C(12A)	122.37(16)	122.37
C(11)-C(12)-C(10)	126.2(3)	125.39	O(11A)-C(11A)-C(10A)	122.27(16)	122.37
C(11)-C(12)-N(7)	127.3(3)	127.60	C(12A)-C(11A)-C(10A)	115.36(15)	115.23
C(10)-C(12)-N(7)	106.5(3)	107.00	C(1A)-C(12A)-N(4A)	107.35(16)	107.20
C(11)-C(13)-C(1)	125.0(3)	125.39	C(1A)-C(12A)-C(11A)	131.91(17)	131.85
C(11)-C(13)-N(4)	128.0(3)	127.60	N(4A)-C(12A)-C(11A)	120.73(15)	120.16
C(1)-C(13)-N(4)	106.9(3)	107.00			

Table 1: [a] Geometry optimisation performed with 6-31G basis set.

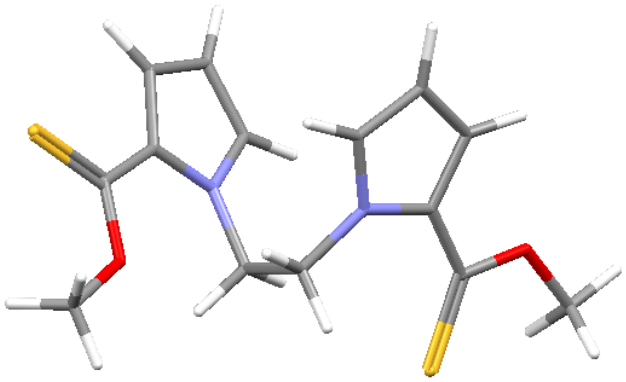
Though the absolute values differ, the trends in the experimental solid-state parameters noted in the Tables above for structures **2** and **3** are almost identical to the MP2 values calculated.

The calculated values for the lengths of the internal C-N bonds of the pyrrole are slightly longer than the external bonds, but the difference is not as pronounced as in the solid state.

The carbonyl bond lengths are: **2**, 1.280 Å; **3**, 1.273 Å; therefore **2** shows a greater level of conjugation than **3**, although once again the difference is not as pronounced as in the crystal structures.

The calculated internal angles at the carbonyls are exactly the same as in the crystal structures.

Table 14. Gas-phase structure of 7 calculated at MP2 level using the 6-31G basis set.[2]



C	2.521284	-1.971850	-1.014747
C	2.326704	-0.609064	-0.673281
N	1.012521	-0.267937	-1.069611
C	0.404163	-1.397687	-1.616016
C	1.322399	-2.458153	-1.595679
C	0.250190	0.978093	-0.824311
C	3.317567	0.289111	-0.101806
N	-0.963660	-0.101450	1.066471
C	-0.366645	-1.162615	1.744112
C	-1.298257	-2.205651	1.860602
C	-2.493078	-1.780813	1.227981
C	-2.281281	-0.469966	0.718437
C	-3.271524	0.369406	0.067421
S	-3.177441	2.024058	-0.379651
O	-4.413073	-0.384496	-0.160070
C	-5.601348	0.258082	-0.772833
S	4.900937	-0.158493	0.358091
O	2.833640	1.587088	0.046118
C	3.737875	2.634261	0.589150
C	-0.179348	1.084528	0.652295
H	3.447340	-2.513902	-0.857315
H	-0.627894	-1.357059	-1.948575
H	1.140728	-3.460904	-1.967403
H	-0.639375	0.932489	-1.464010
H	0.851621	1.844987	-1.107939
H	0.669890	-1.097755	2.057826
H	-1.125524	-3.156330	2.353676
H	-3.425842	-2.326000	1.144872
H	-5.354720	0.633469	-1.771146
H	-5.952016	1.082014	-0.143076
H	-6.328651	-0.554331	-0.815993
H	4.612609	2.744106	-0.059162
H	4.057190	2.366527	1.601236
H	3.115893	3.531433	0.584501
H	-0.766921	1.992481	0.812649
H	0.710958	1.108606	1.290476

Table 15. Crystal data and structure refinement for 8 (hm8001).

Contact Simon Parsons, s.parsons@ed.ac.uk

A. CRYSTAL DATA

Empirical formula C13 H14 N2 O2 S2
C13 H14 N2 O2 S2
Formula weight 294.38
Wavelength 0.71073 A
Temperature 150(2) K
Crystal system Triclinic
Space group P-1

Unit cell dimensions a = 8.0365(2) A alpha = 98.8420(10) deg.

b = 8.9123(2) A beta = 107.7310(10) deg.

c = 11.2816(3) A gamma = 111.5210(10) deg.
Volume 683.11(3) A^3
Number of reflections for cell 8646 (2.5 < theta < 30 deg.)
Z 2
Density (calculated) 1.431 Mg/m^3
Absorption coefficient 0.388 mm^-1
F(000) 308

B. DATA COLLECTION
Crystal description orange block
Crystal size 0.45 x 0.37 x 0.26 mm
Instrument Bruker Smart APEX CCD
Theta range for data collection 1.99 to 29.97 deg.
Index ranges -11<=h<=9, -12<=k<=12, -15<=l<=15
Reflections collected 11638
Independent reflections 3705 [R(int) = 0.0269]
Scan type omega and phi
Absorption correction Multiscan
(Tmin= 0.753, Tmax=0.903)

C. SOLUTION AND REFINEMENT.
Solution Patterson (DIRDIF)
Refinement type Full-matrix least-squares on F^2
Program used for refinement SHELXL-97
Hydrogen atom placement geom
Hydrogen atom treatment riding
Data / restraints / parameters 3705/5/201
Goodness-of-fit on F^2 1.145
Conventional R [F>4sigma(F)] R1 = 0.0481 [3502 data]
Weighted R (F^2 and all data) wR2 = 0.1180
Extinction coefficient 0.018(3)
Final maximum delta/sigma 0.000
Weighting scheme
calc w=1/[\s^2^(Fo^2^)+(0.0469P)^2^+0.3545P] where P=(Fo^2^+2Fc^2^)/3
Largest diff. peak and hole 0.425 and -0.300 e.A^-3

Table 16. Atomic coordinates (x 10^4), equivalent isotropic displacement parameters (A^2 x 10^3) and site occupancies for 8 (hm8001). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	Occ
N(1)	8816(2)	-1673(2)	3166(1)	26(1)	1
C(2)	9096(2)	-2386(2)	4185(1)	25(1)	1
C(3)	10491(2)	-2953(2)	4170(2)	30(1)	1
C(4)	11038(3)	-2598(2)	3145(2)	35(1)	1
C(5)	9996(2)	-1814(2)	2549(2)	31(1)	1
C(6)	7576(2)	-857(2)	2770(2)	28(1)	1
C(7)	8095(2)	-2537(2)	5061(2)	27(1)	1
S(8)	6272(1)	-2160(1)	5017(1)	34(1)	0.80(1)
O(9)	8994(3)	-3131(3)	5998(2)	32(1)	0.80(1)
C(10)	8219(4)	-3455(3)	6988(2)	36(1)	0.80(1)
S(8')	8252(6)	-3313(4)	6187(3)	42(1)	0.20(1)
O(9')	6821(11)	-1732(11)	4679(7)	40(2)	0.20(1)
C(10')	5613(14)	-1766(14)	5418(10)	46(3)	0.20(1)
N(1A)	5601(2)	-2109(2)	1856(1)	25(1)	1
C(2A)	4066(2)	-1782(2)	1193(1)	26(1)	1
C(3A)	2495(2)	-3342(2)	449(2)	33(1)	1
C(4A)	3069(3)	-4602(2)	659(2)	35(1)	1
C(5A)	4990(3)	-3804(2)	1527(2)	32(1)	1
C(7A)	4140(2)	-129(2)	1271(2)	28(1)	1
S(8A)	2309(1)	189(1)	399(1)	42(1)	1
O(9A)	5835(2)	1101(2)	2133(1)	33(1)	1
C(10A)	6162(3)	2833(2)	2302(2)	40(1)	1

Table 17. Bond lengths [Å] and angles [deg] for 8 (hm8001).

N(1)-C(5)	1.364(2)
N(1)-C(2)	1.3959(19)
N(1)-C(6)	1.443(2)
C(2)-C(3)	1.391(2)
C(2)-C(7)	1.445(2)
C(3)-C(4)	1.397(2)
C(4)-C(5)	1.368(2)
C(6)-N(1A)	1.475(2)
C(7)-O(9)	1.381(2)
C(7)-O(9')	1.454(6)
C(7)-S(8')	1.531(3)
C(7)-S(8)	1.6082(17)
O(9)-C(10)	1.453(3)
O(9')-C(10')	1.455(8)
N(1A)-C(5A)	1.354(2)
N(1A)-C(2A)	1.391(2)
C(2A)-C(3A)	1.392(2)
C(2A)-C(7A)	1.440(2)
C(3A)-C(4A)	1.387(3)
C(4A)-C(5A)	1.381(2)
C(7A)-O(9A)	1.331(2)
C(7A)-S(8A)	1.6498(16)
O(9A)-C(10A)	1.439(2)
C(5)-N(1)-C(2)	108.49(13)
C(5)-N(1)-C(6)	121.82(14)
C(2)-N(1)-C(6)	129.67(14)
C(3)-C(2)-N(1)	106.60(14)
C(3)-C(2)-C(7)	126.95(14)
N(1)-C(2)-C(7)	126.44(14)
C(2)-C(3)-C(4)	108.32(15)
C(5)-C(4)-C(3)	107.25(15)
N(1)-C(5)-C(4)	109.34(15)
N(1)-C(6)-N(1A)	110.81(12)
O(9)-C(7)-C(2)	106.23(16)
O(9)-C(7)-O(9')	147.4(3)
C(2)-C(7)-O(9')	105.1(3)
O(9)-C(7)-S(8')	25.82(12)
C(2)-C(7)-S(8')	131.1(2)
O(9')-C(7)-S(8')	123.8(3)
O(9)-C(7)-S(8)	123.91(15)
C(2)-C(7)-S(8)	129.85(13)
O(9')-C(7)-S(8)	26.3(3)
S(8')-C(7)-S(8)	98.63(18)
C(7)-O(9)-C(10)	117.68(19)
C(7)-O(9')-C(10')	115.0(7)
C(5A)-N(1A)-C(2A)	108.44(14)
C(5A)-N(1A)-C(6)	124.47(14)
C(2A)-N(1A)-C(6)	127.09(13)
N(1A)-C(2A)-C(3A)	106.86(14)
N(1A)-C(2A)-C(7A)	125.46(14)
C(3A)-C(2A)-C(7A)	127.67(15)
C(4A)-C(3A)-C(2A)	108.39(15)
C(5A)-C(4A)-C(3A)	106.84(16)
N(1A)-C(5A)-C(4A)	109.47(16)
O(9A)-C(7A)-C(2A)	112.45(13)
O(9A)-C(7A)-S(8A)	124.13(13)

C(2A)-C(7A)-S(8A)	123.42(13)
C(7A)-O(9A)-C(10A)	119.38(14)

Symmetry transformations used to generate equivalent atoms:

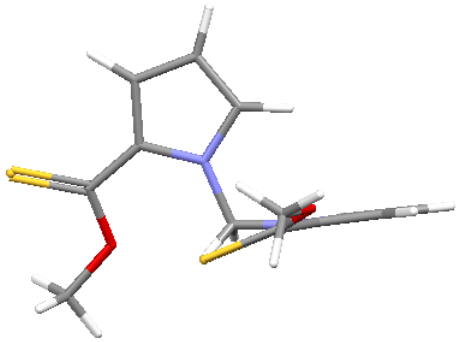
Table 18. Anisotropic displacement parameters (A^2 x 10^3) for 8 (hm8001). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	25(1)	26(1)	26(1)	9(1)	7(1)	12(1)
C(2)	24(1)	24(1)	24(1)	7(1)	7(1)	11(1)
C(3)	30(1)	31(1)	31(1)	10(1)	10(1)	17(1)
C(4)	34(1)	39(1)	37(1)	11(1)	17(1)	21(1)
C(5)	31(1)	33(1)	28(1)	10(1)	13(1)	12(1)
C(6)	26(1)	22(1)	30(1)	7(1)	2(1)	10(1)
C(7)	25(1)	23(1)	27(1)	3(1)	7(1)	7(1)
S(8)	30(1)	45(1)	36(1)	13(1)	15(1)	23(1)
O(9)	34(1)	44(1)	31(1)	20(1)	18(1)	22(1)
C(10)	40(1)	44(1)	30(1)	17(1)	18(1)	19(1)
S(8')	53(2)	43(1)	41(2)	24(1)	21(1)	24(1)
O(9')	42(4)	58(5)	39(4)	22(3)	32(3)	27(4)
C(10')	42(5)	49(6)	39(5)	7(4)	19(5)	11(5)
N(1A)	25(1)	23(1)	24(1)	7(1)	6(1)	9(1)
C(2A)	22(1)	33(1)	23(1)	9(1)	9(1)	12(1)
C(3A)	24(1)	41(1)	27(1)	7(1)	9(1)	8(1)
C(4A)	32(1)	29(1)	33(1)	1(1)	12(1)	4(1)
C(5A)	34(1)	23(1)	33(1)	6(1)	9(1)	10(1)
C(7A)	29(1)	38(1)	28(1)	16(1)	16(1)	19(1)
S(8A)	38(1)	63(1)	43(1)	27(1)	16(1)	34(1)
O(9A)	33(1)	27(1)	41(1)	13(1)	12(1)	17(1)
C(10A)	52(1)	30(1)	53(1)	19(1)	27(1)	25(1)

Table 19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 8 (hm8001).

	x	y	z	U(eq)	Occ
H(3)	10986	-3490	4757	36	1
H(4)	11961	-2854	2906	42	1
H(5)	10080	-1429	1820	37	1
H(6A)	8136	-24	2344	34	1
H(6B)	7505	-241	3548	34	1
H(10A)	8983	-3869	7589	54	0.80(1)
H(10B)	6860	-4309	6570	54	0.80(1)
H(10C)	8292	-2407	7475	54	0.80(1)
H(10D)	4837	-1168	5116	69	0.20(1)
H(10E)	6444	-1213	6347	69	0.20(1)
H(10F)	4745	-2942	5289	69	0.20(1)
H(3A)	1244	-3513	-108	40	1
H(4A)	2289	-5786	280	42	1
H(5A)	5764	-4358	1843	38	1
H(10G)	7468	3580	2966	60	1
H(10H)	5192	3014	2582	60	1
H(10I)	6050	3086	1474	60	1

Table 20. Gas-phase structure of 8 calculated at MP2 level using the 6-31G basis set.[2]



C	1.973949	-0.419334	2.313623
C	1.883104	-0.381359	0.902043
N	0.629026	-0.927185	0.551252
C	-0.049085	-1.291039	1.717796
C	0.771135	-0.983067	2.814019
C	0.061251	-1.063648	-0.819884
C	2.901160	0.055713	-0.038358
N	-1.381525	-1.300842	-0.744029
C	-1.927616	-2.588380	-0.820746
C	-3.295956	-2.506364	-0.542969
C	-3.595824	-1.140471	-0.267360
C	-2.400758	-0.394203	-0.387512
C	-2.249347	1.048328	-0.229063
S	-0.993184	2.061932	-0.785057
O	-3.360945	1.534900	0.439034
C	-3.490294	2.997484	0.656601
S	4.296678	0.949787	0.361789
O	2.609483	-0.359076	-1.334826
C	3.525487	0.031652	-2.436623
H	2.830537	-0.071379	2.880700
H	-1.047773	-1.709793	1.681509
H	0.518063	-1.153067	3.855201
H	0.511008	-1.920818	-1.332044
H	0.262884	-0.154244	-1.379819
H	-1.296294	-3.436795	-1.062538
H	-3.995993	-3.334962	-0.552497
H	-4.563335	-0.713873	-0.029833
H	-3.508461	3.521809	-0.304663
H	-2.653685	3.360197	1.262136
H	-4.440713	3.088701	1.184633
H	4.518736	-0.393888	-2.263268
H	3.592759	1.122501	-2.497468
H	3.052320	-0.394180	-3.323406

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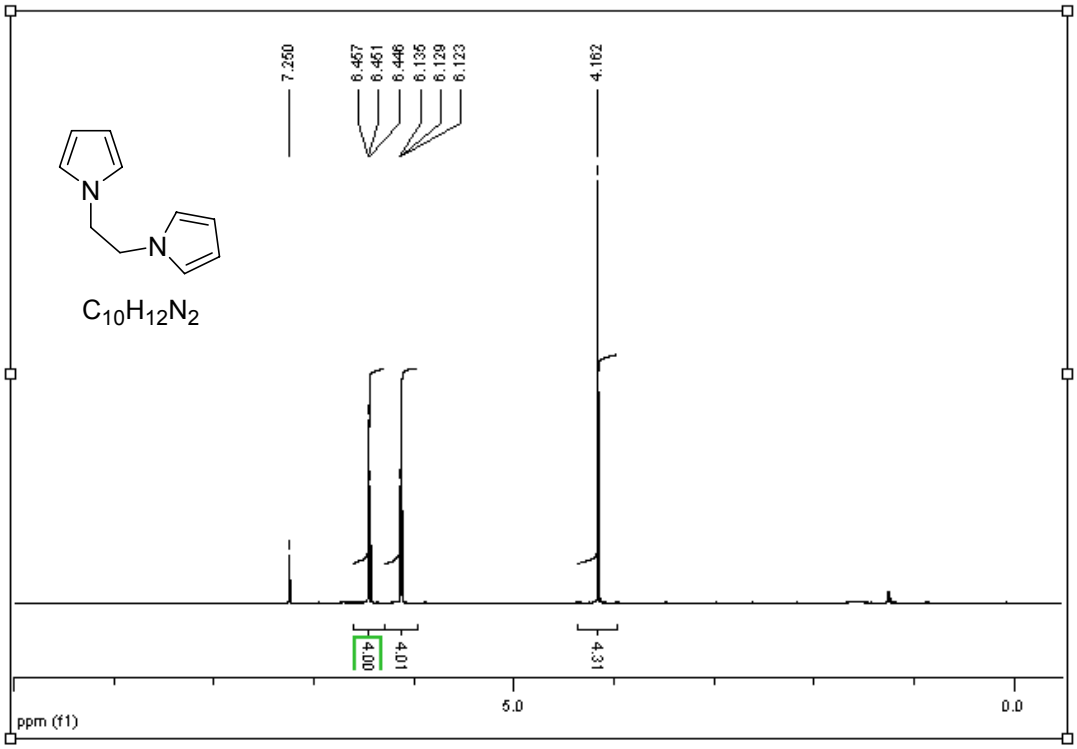
1. U. Burger and F. Dreier, *Tetrahedron*, 1983, **39**, 2065-2071.
2. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, I.; R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian03; Gaussian, Inc., Wallingford CT, 2004.

1,2-Di(pyrrol-1-yl)ethane 4

^{1}H



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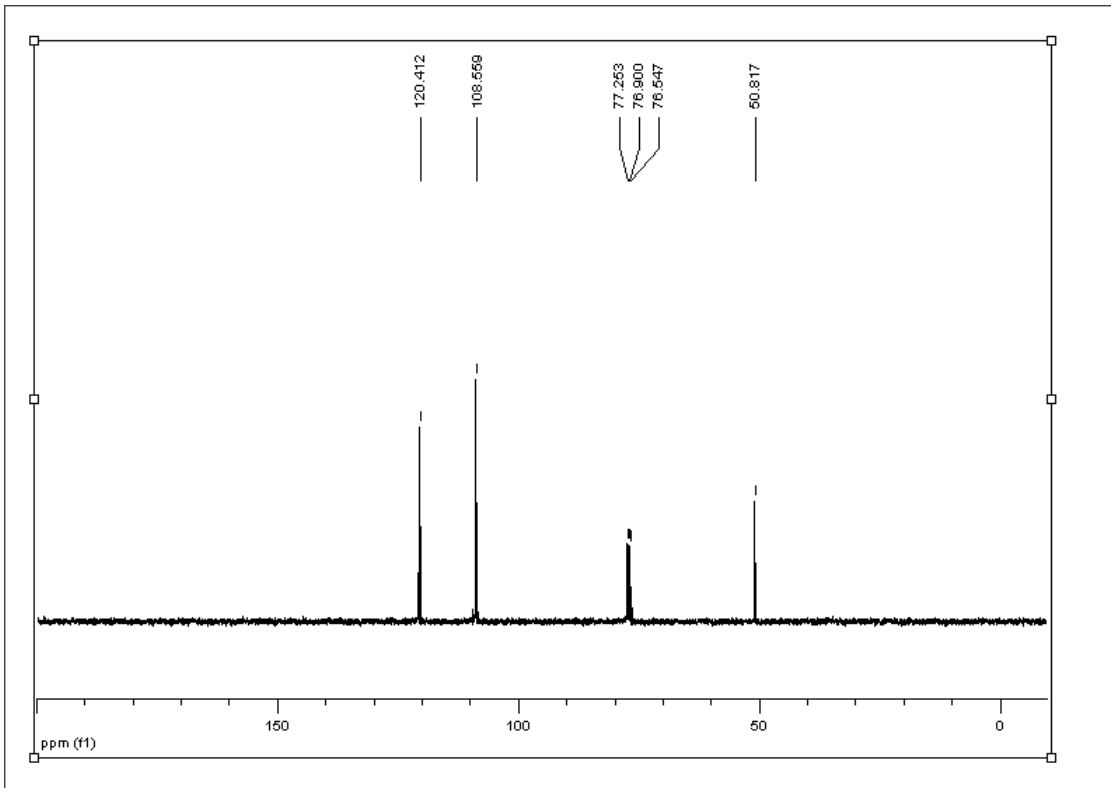

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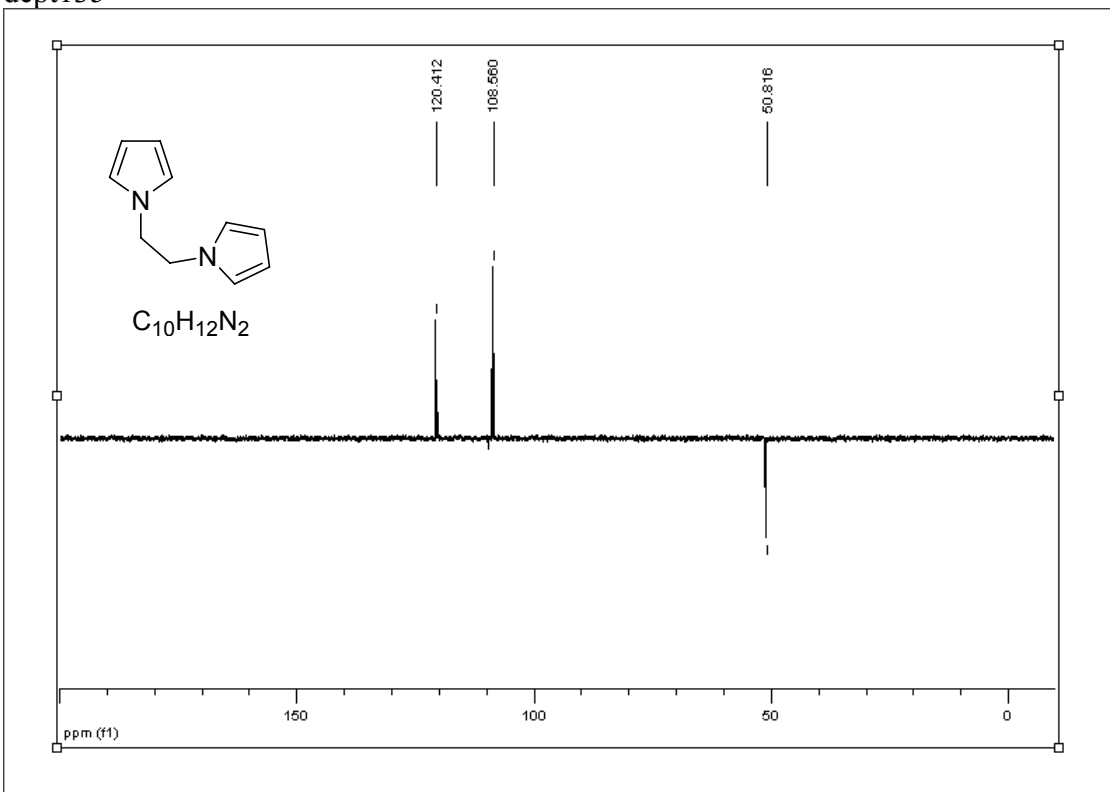

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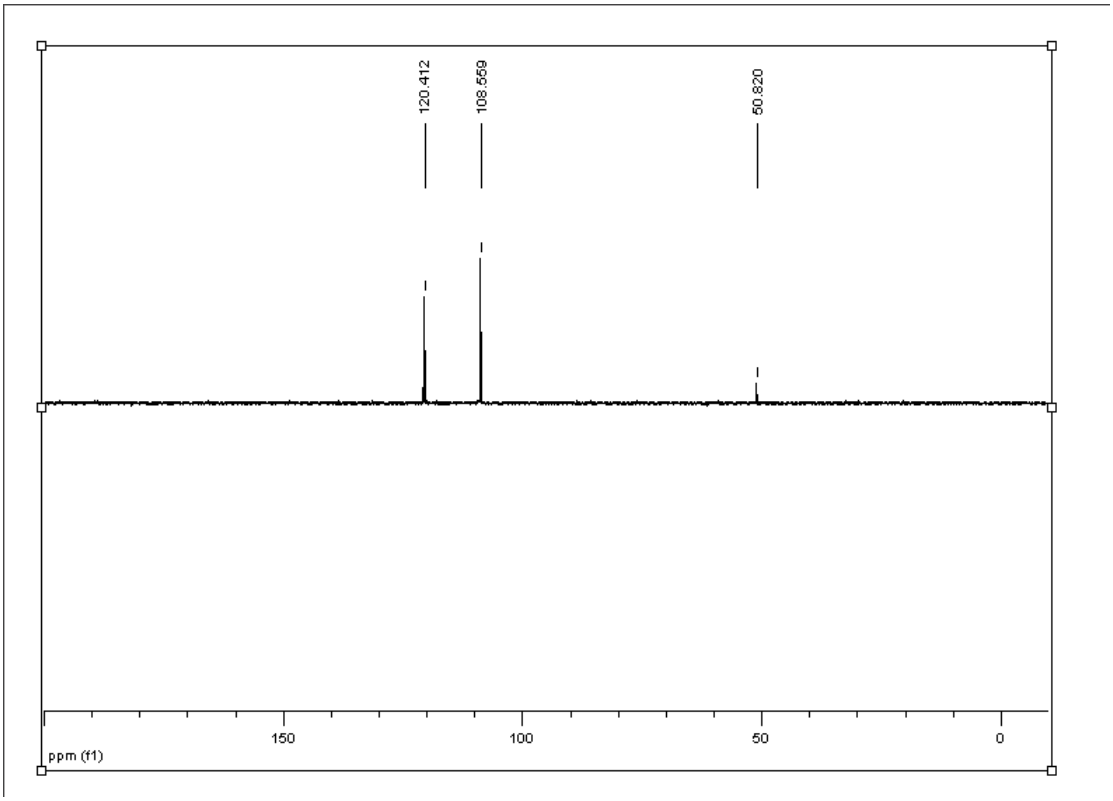
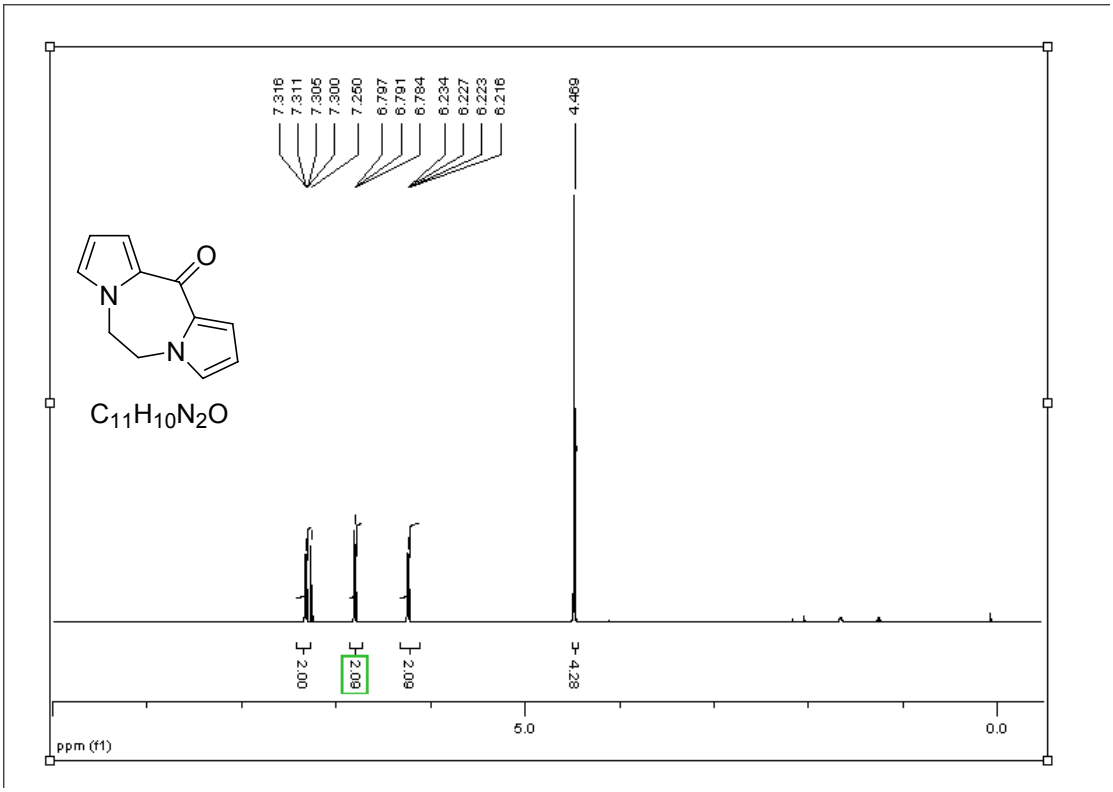


5,6-Dihydrodipyrrolo[1,2-*d*;1′,2′-*g*][1,4]diazepin-11-one 2

^{1}H



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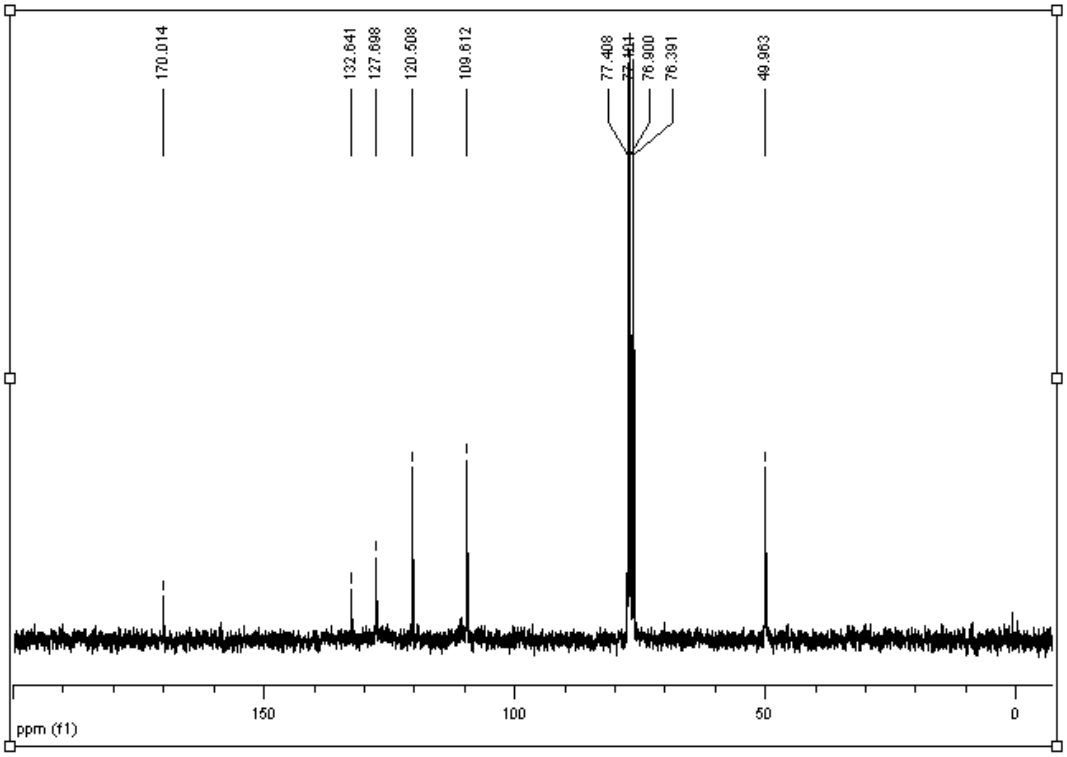

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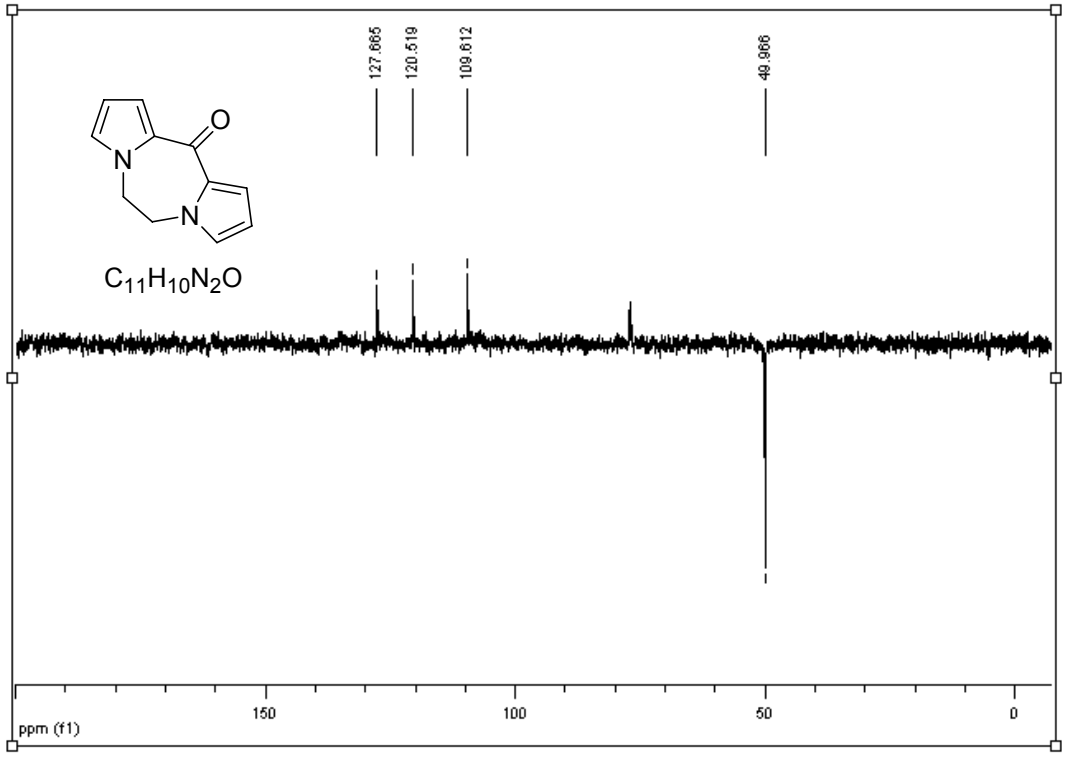

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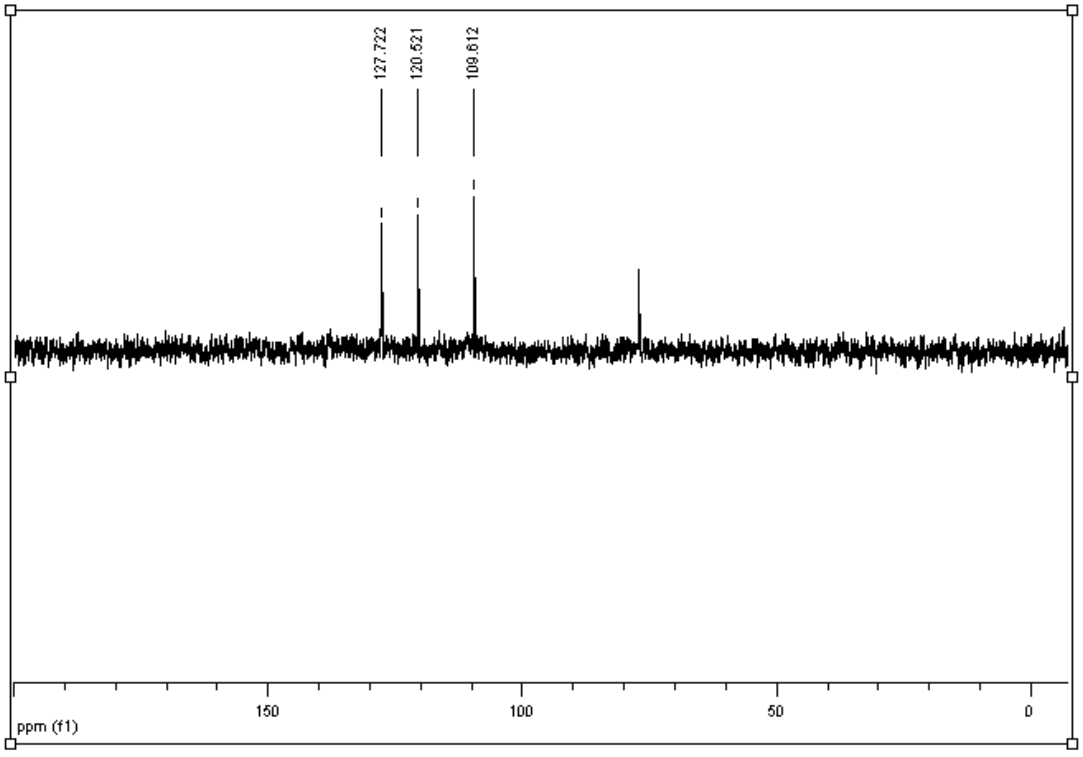
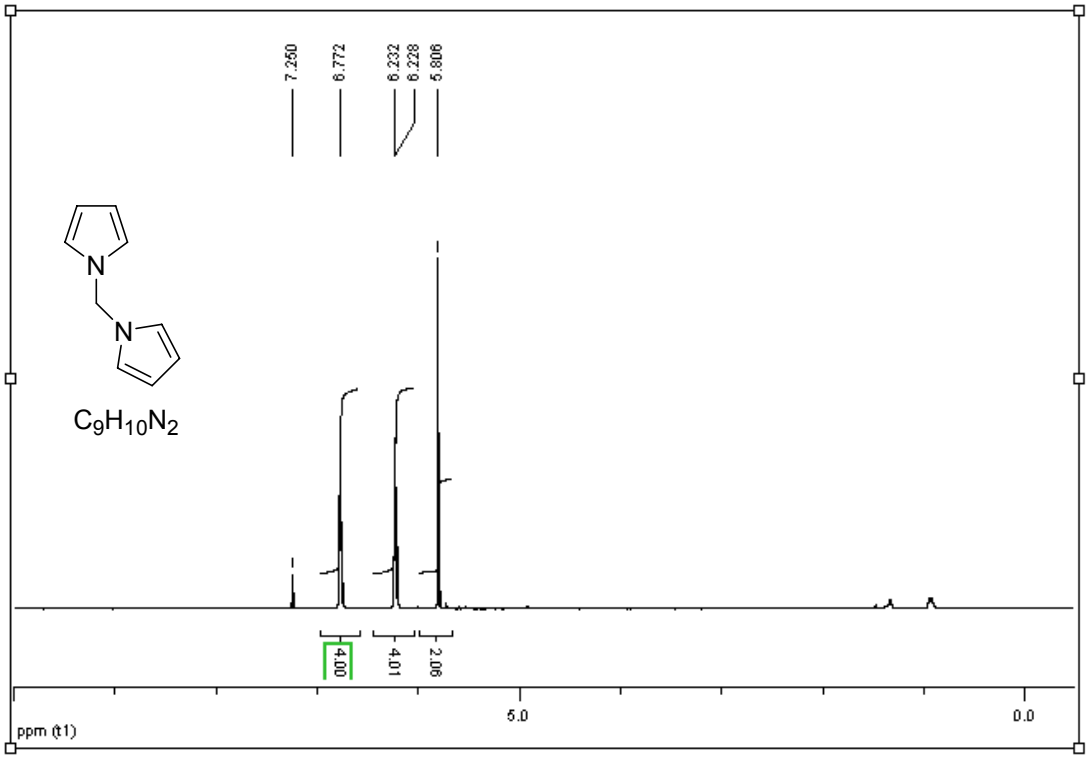


1,1-Di(pyrrol-1-yl)methane 5

^{1}H



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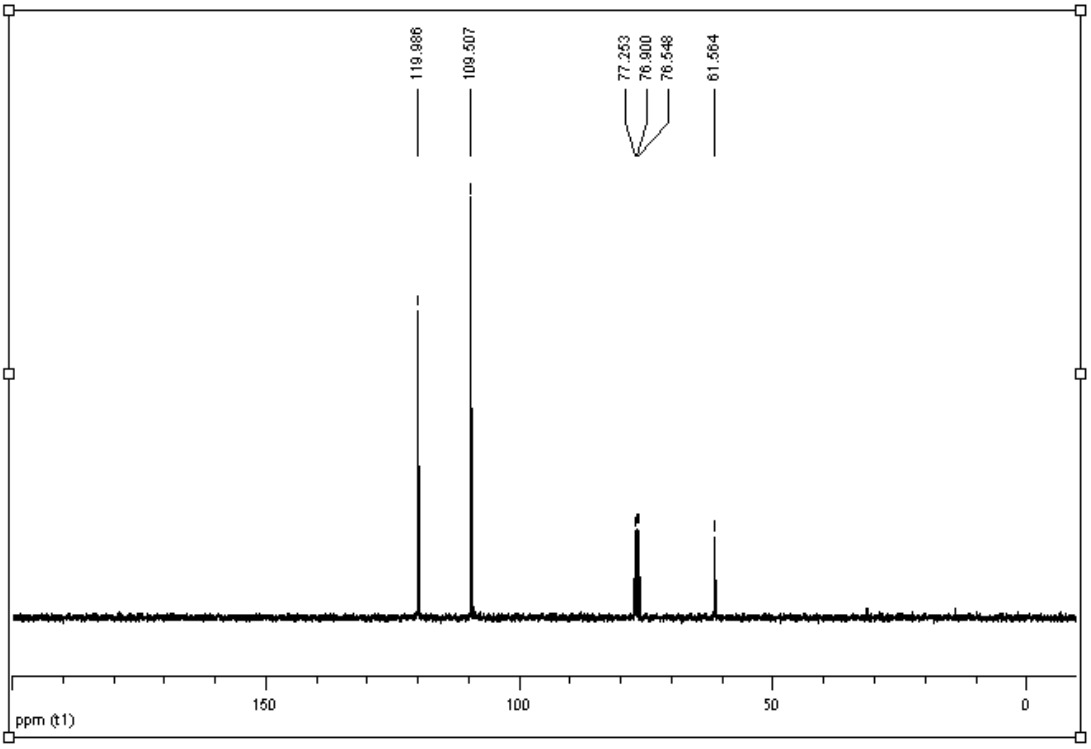

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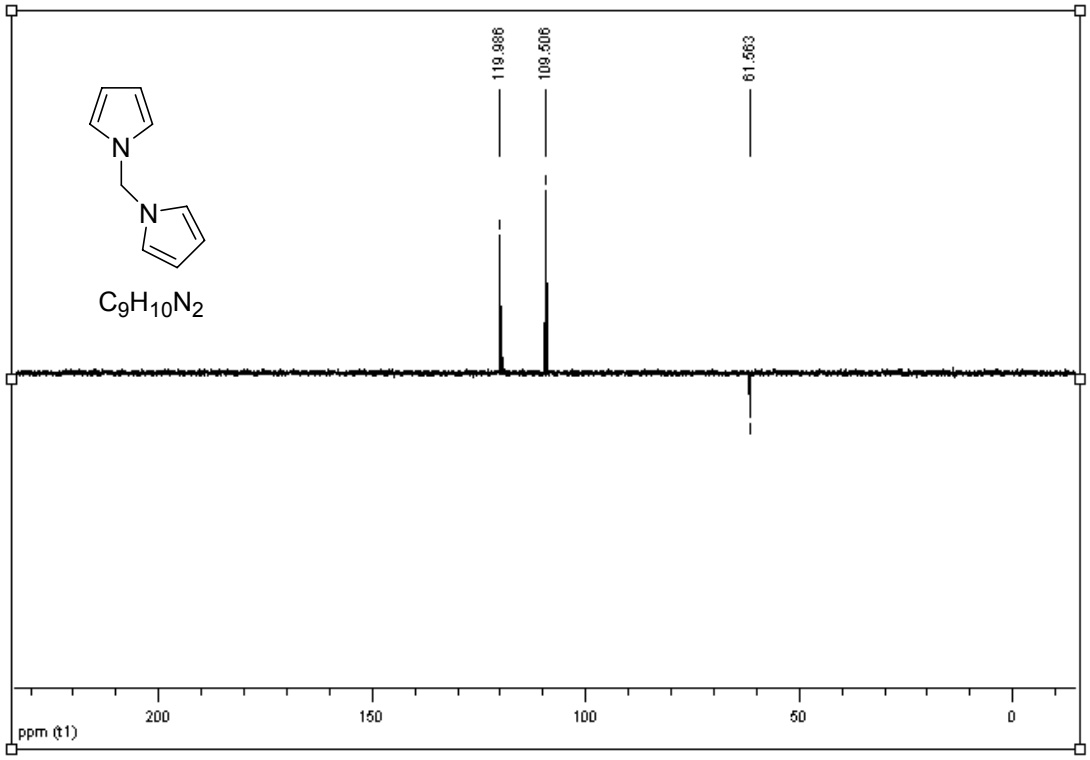

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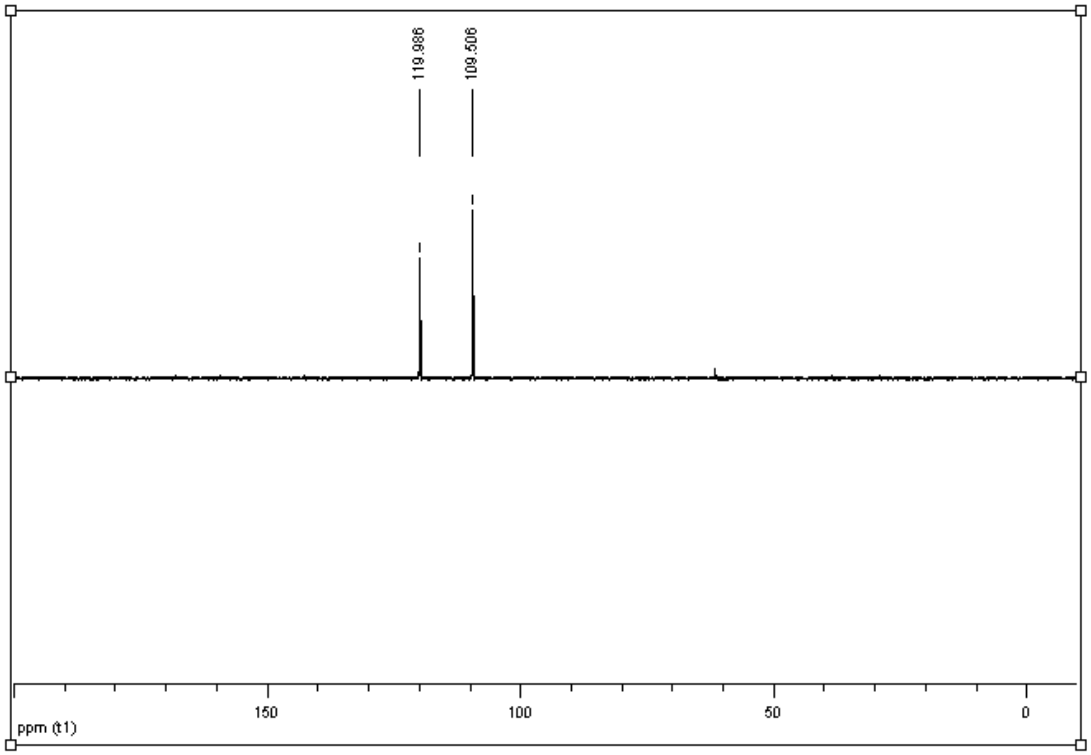
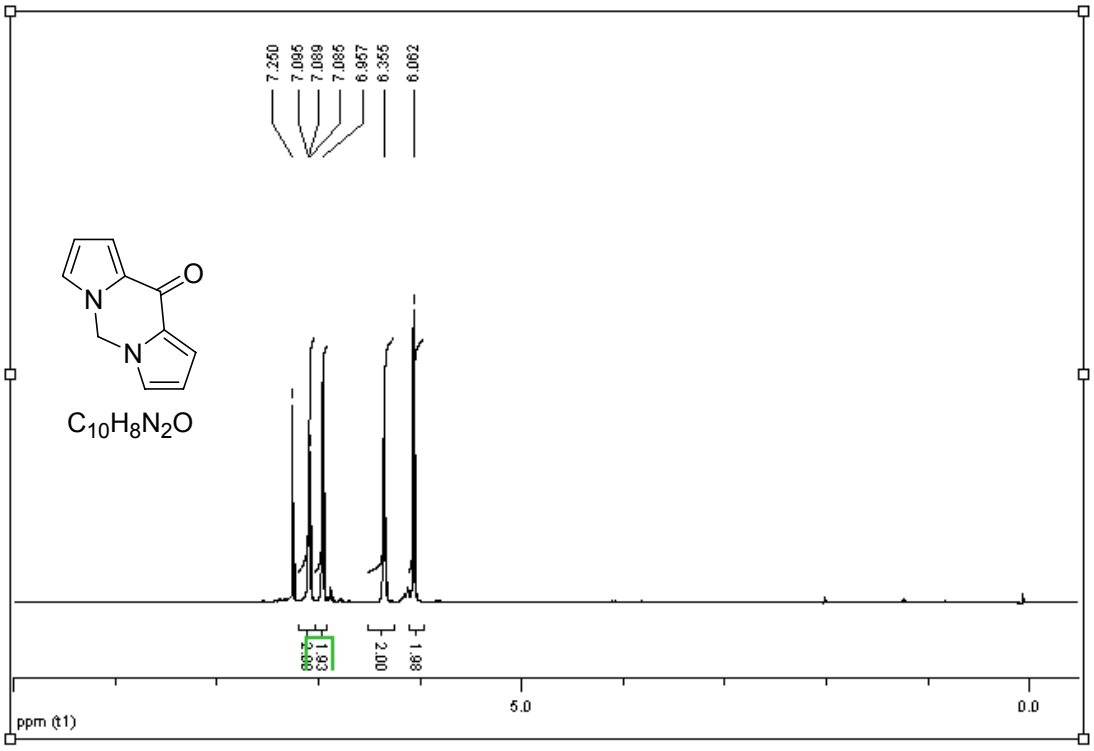


Dipyrrolo[1,2-*c*;1′,2′-*f*]pyrimidin-10-one 3

^{1}H



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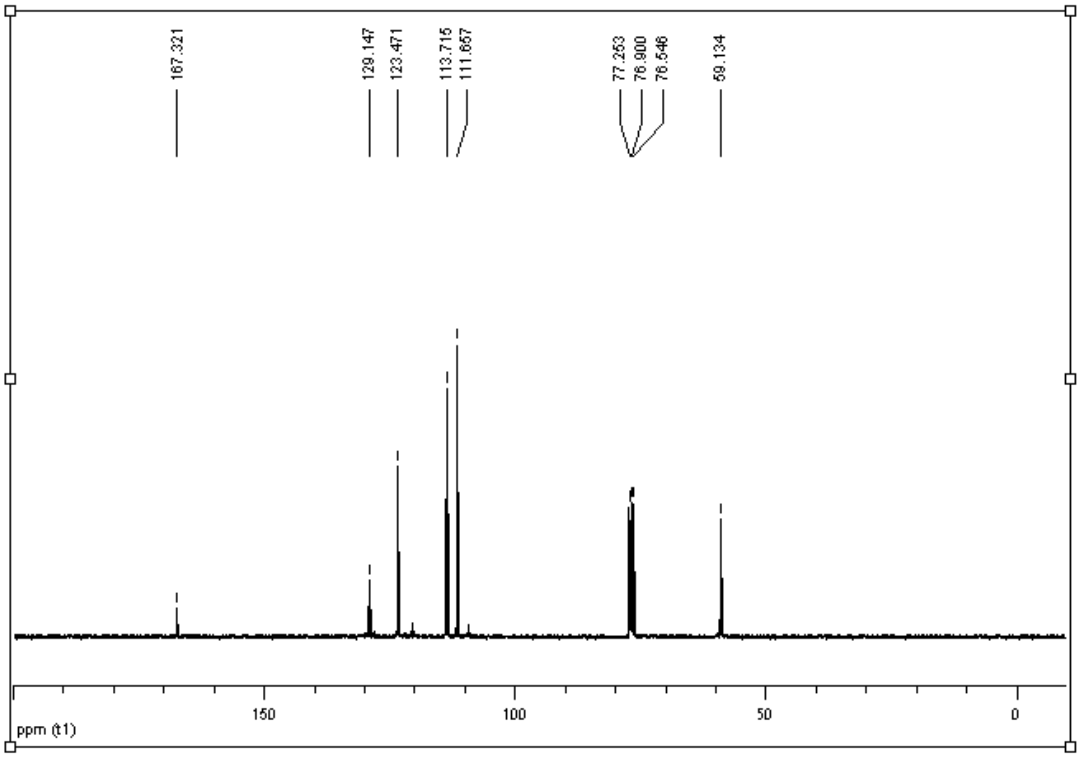

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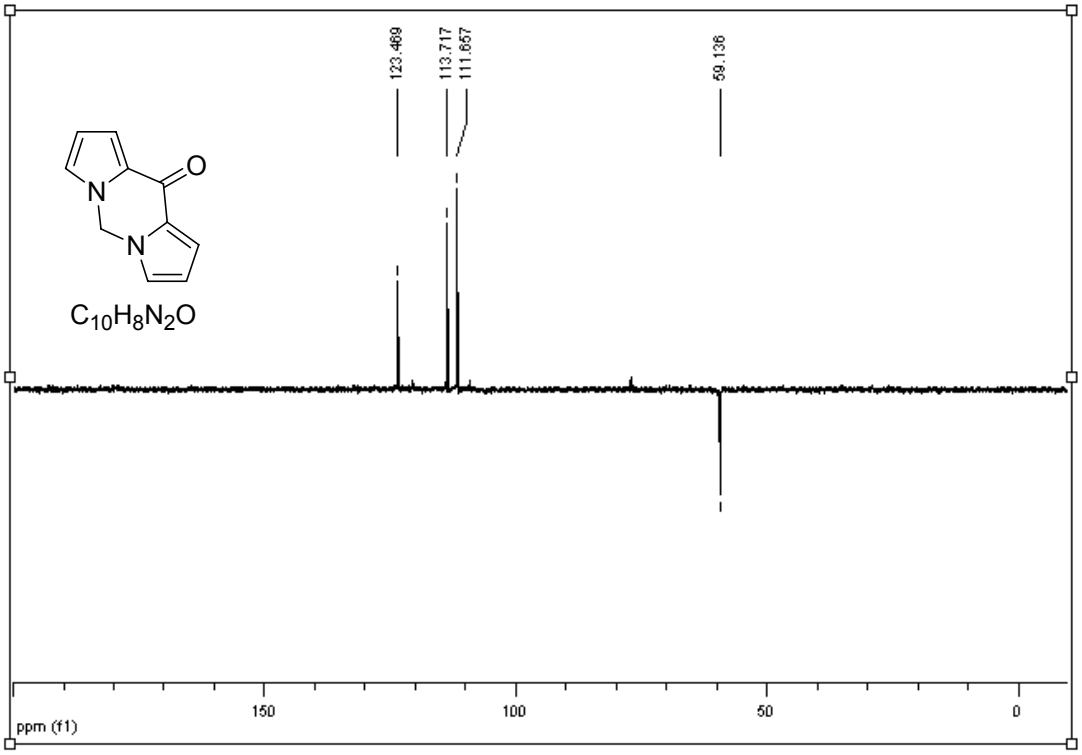

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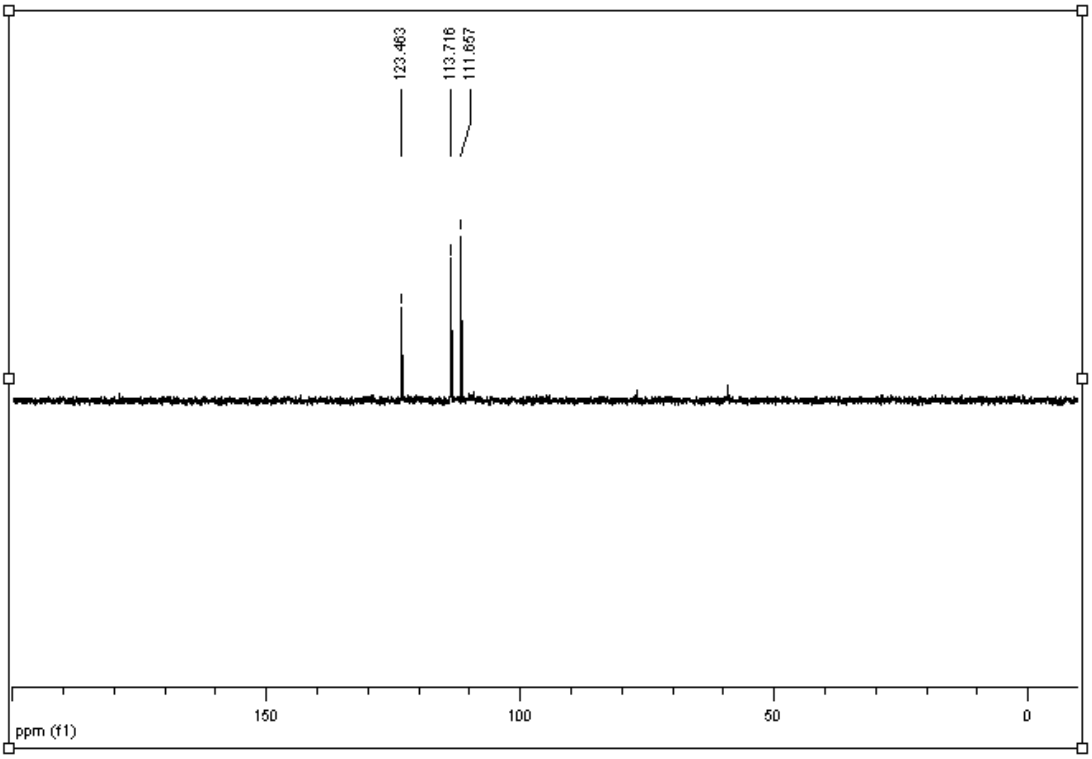
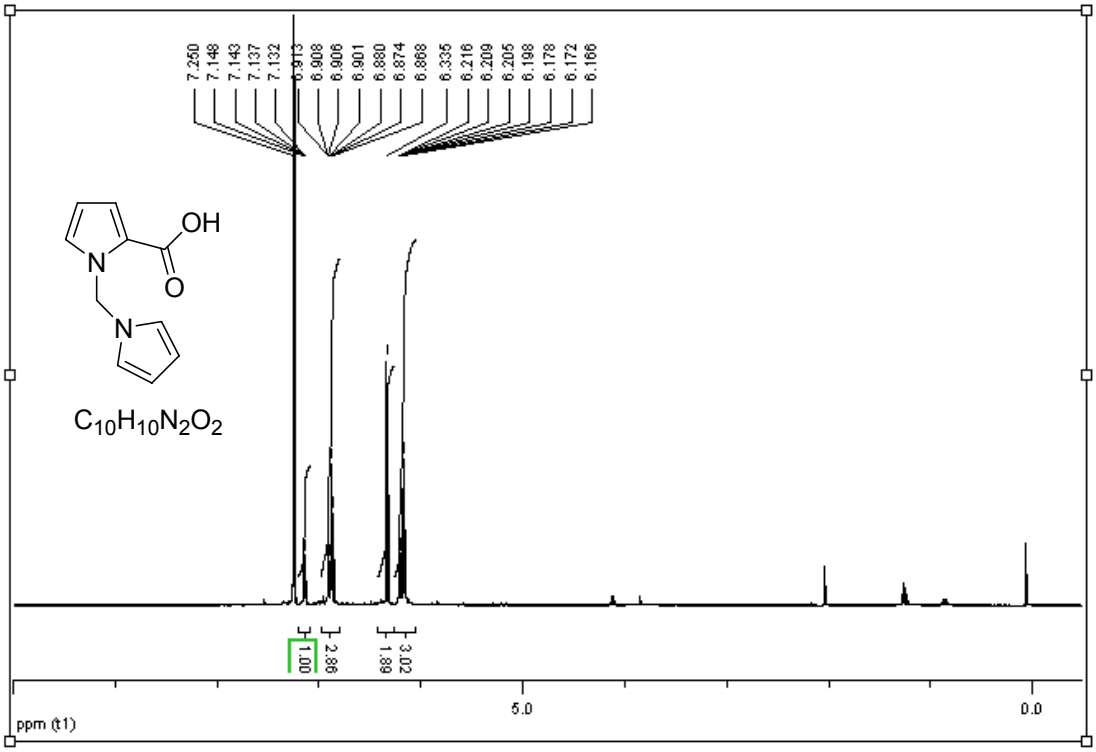
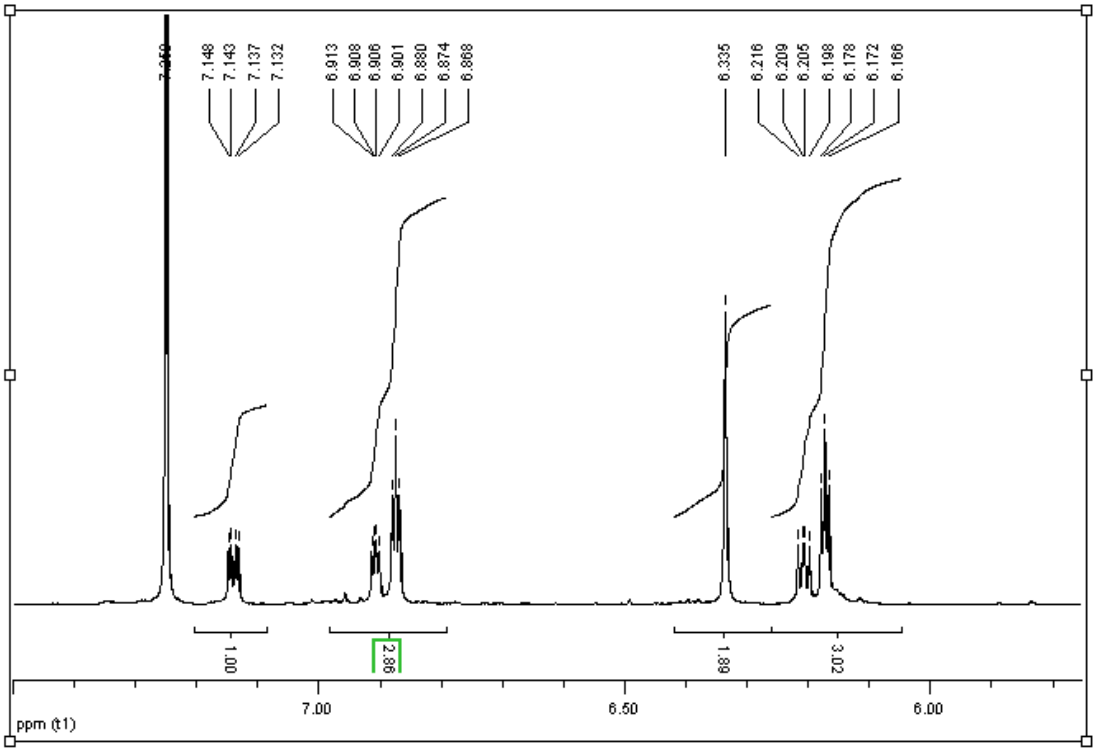


1-(Pyrrol-1-yl)-1-(2-carboxypyrrol-1-yl)methane 6

^1H





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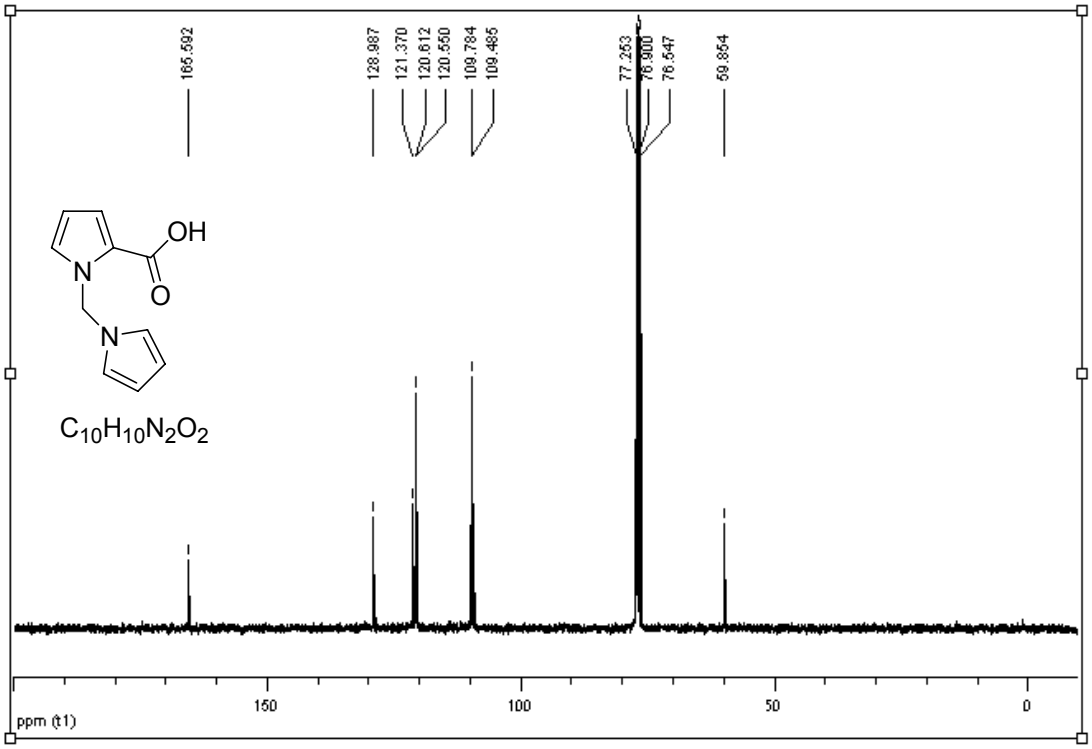
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120.612
120.550
109.784
109.485
77.253
76.900
76.547
59.854
OH
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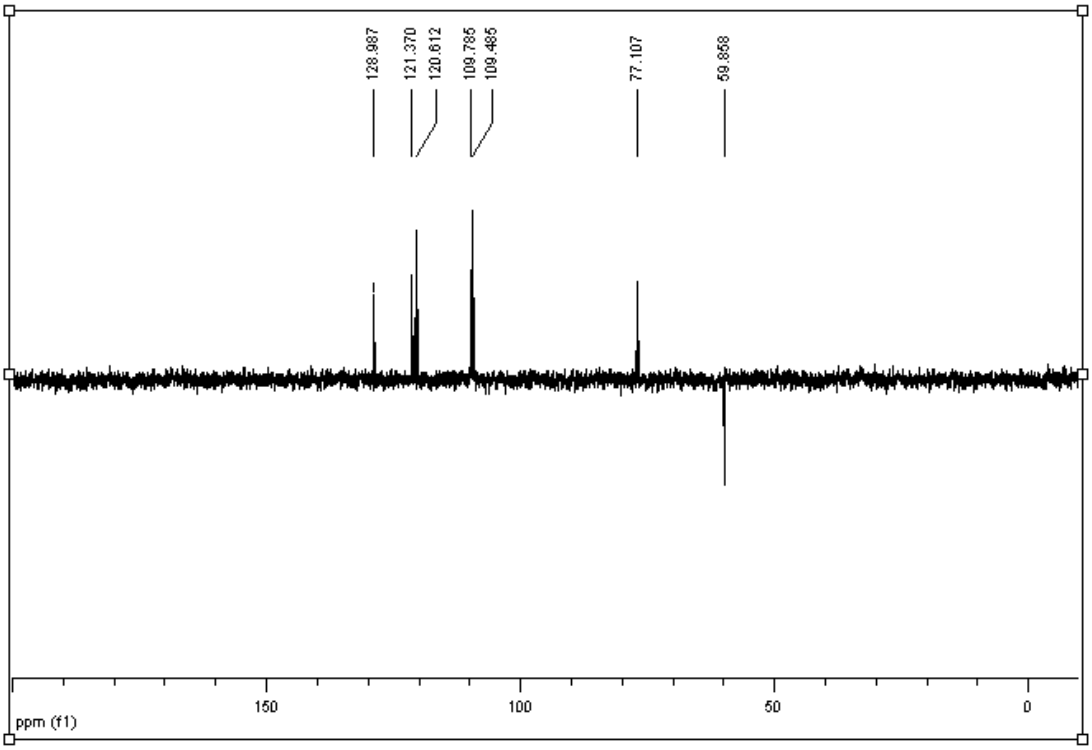
O
N
C10H10N2O2
150
100
50
0
ppm (t1)

dept135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109.785
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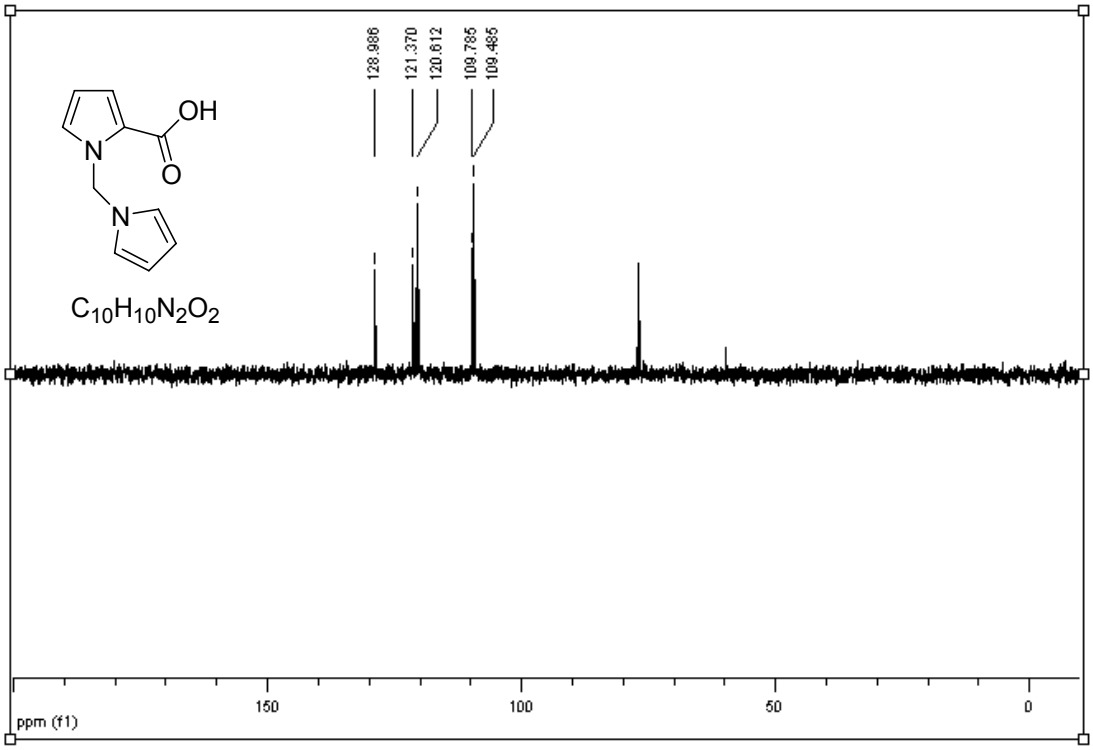
77.107
59.858
150
100
50
0
ppm (f1)

dept90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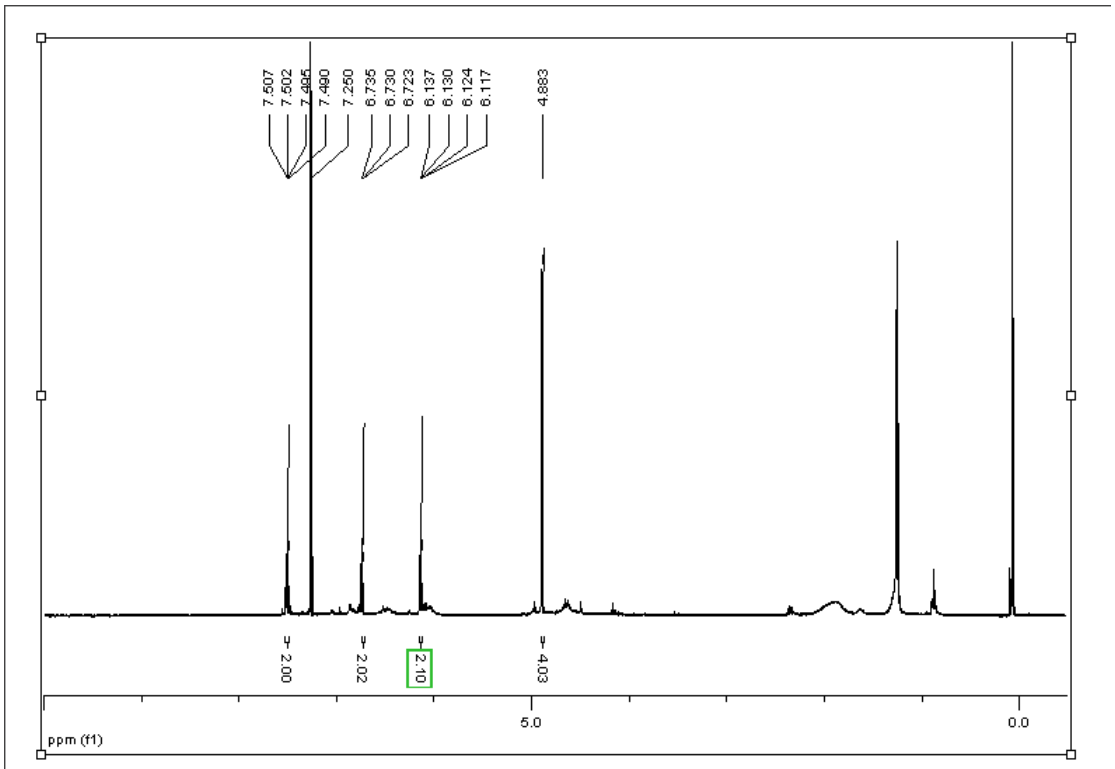
120.612
109.785
109.485
OH
O
N
N
$C_{10}H_{10}N_2O_2$
150
100
50
0
ppm (f1)

Initial product from the reaction of thiophosgene with 1,2-di(pyrrol-1-yl)ethane

^{1}H



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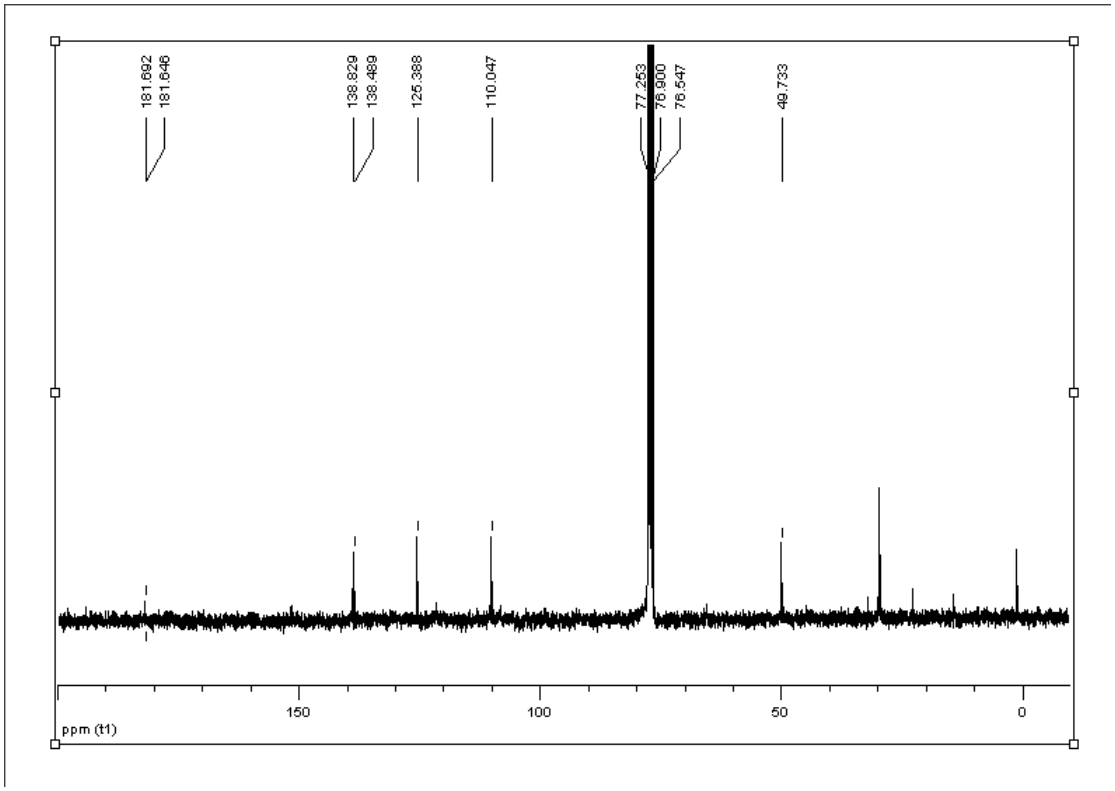
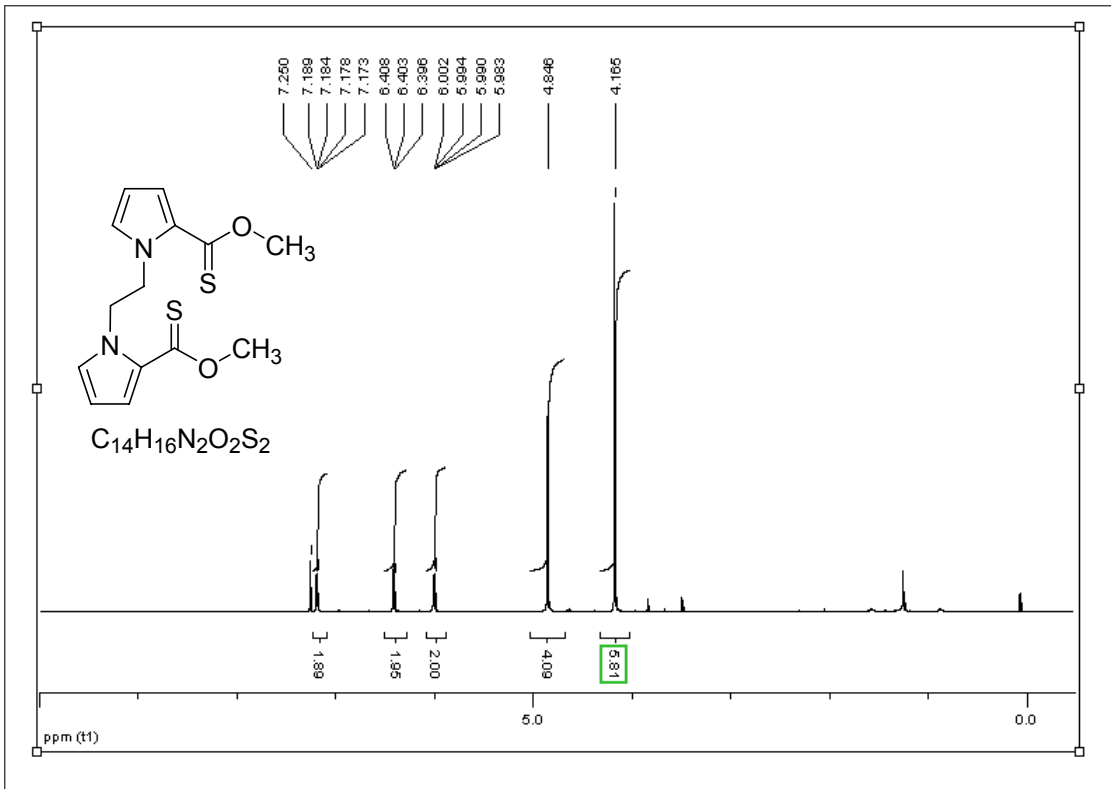


1,2-Di[2-(carbothiomethoxy)pyrrol-1-yl]ethane 7

^{1}H



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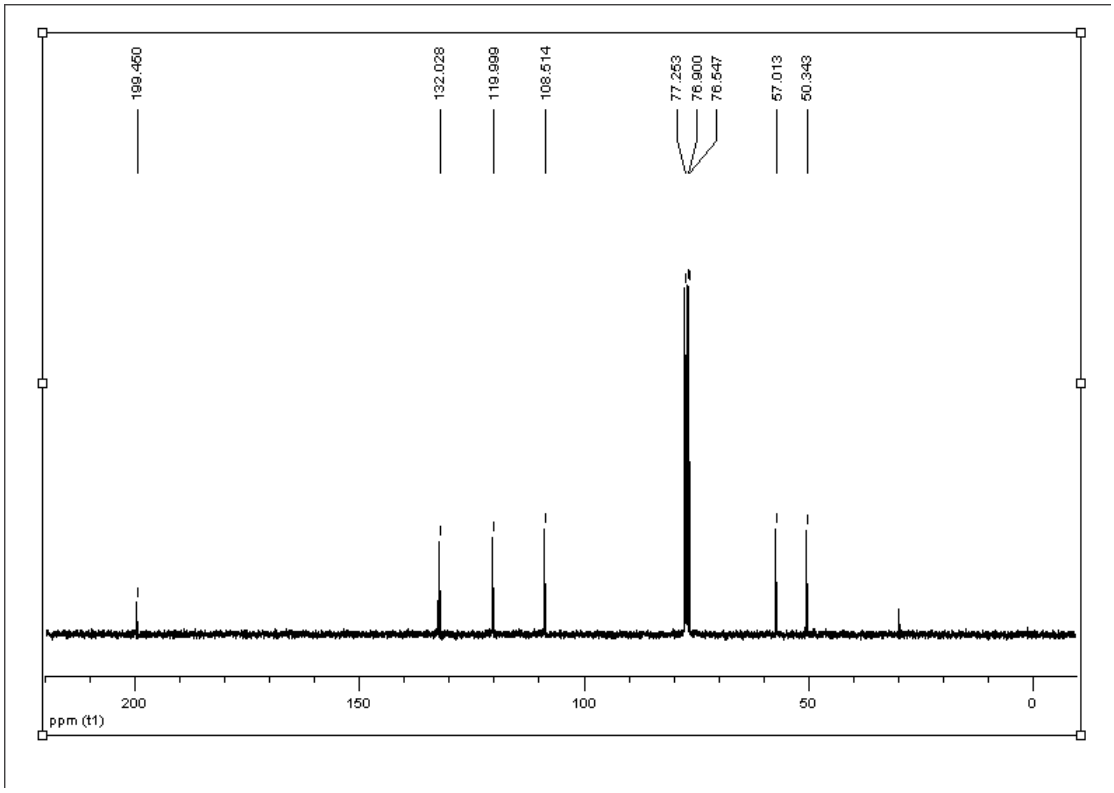

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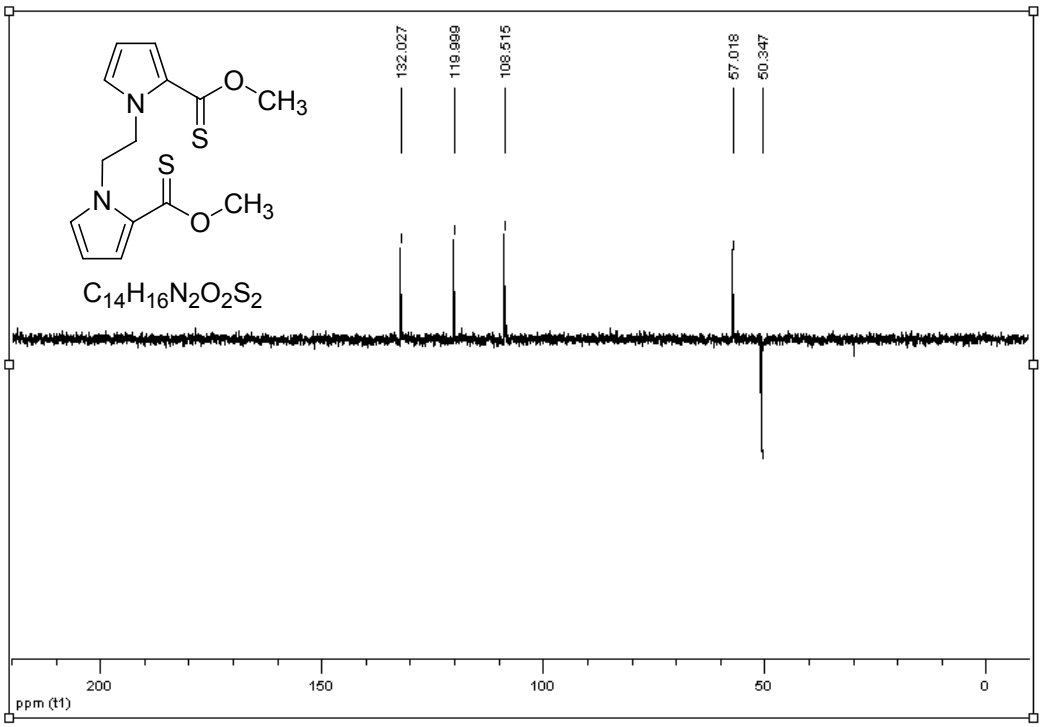

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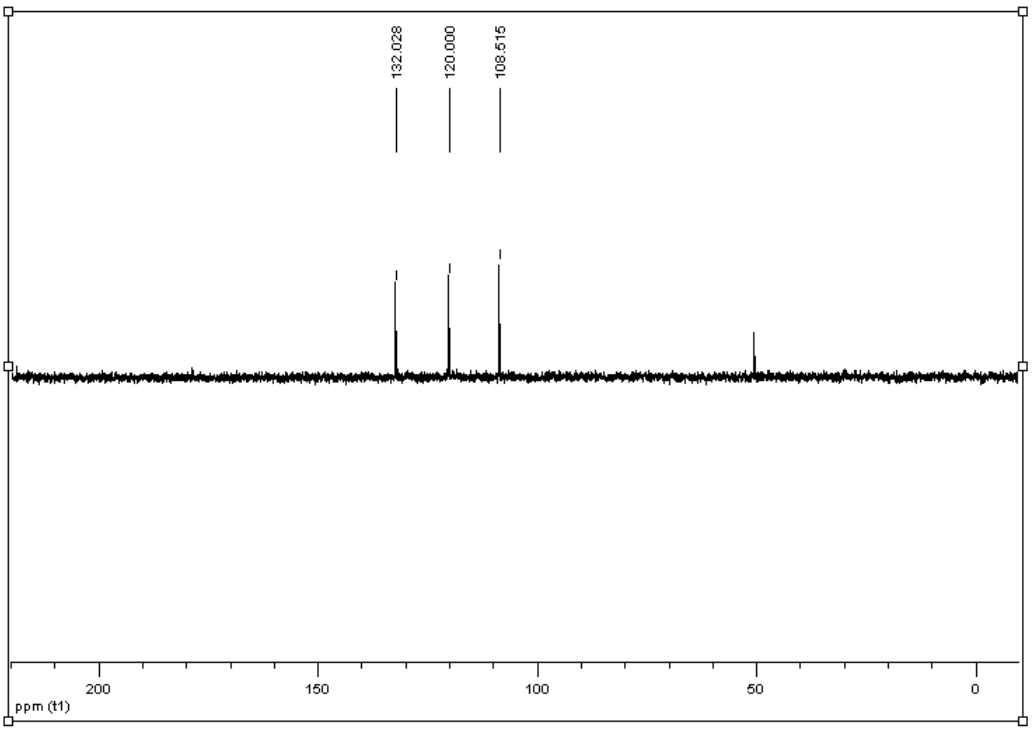
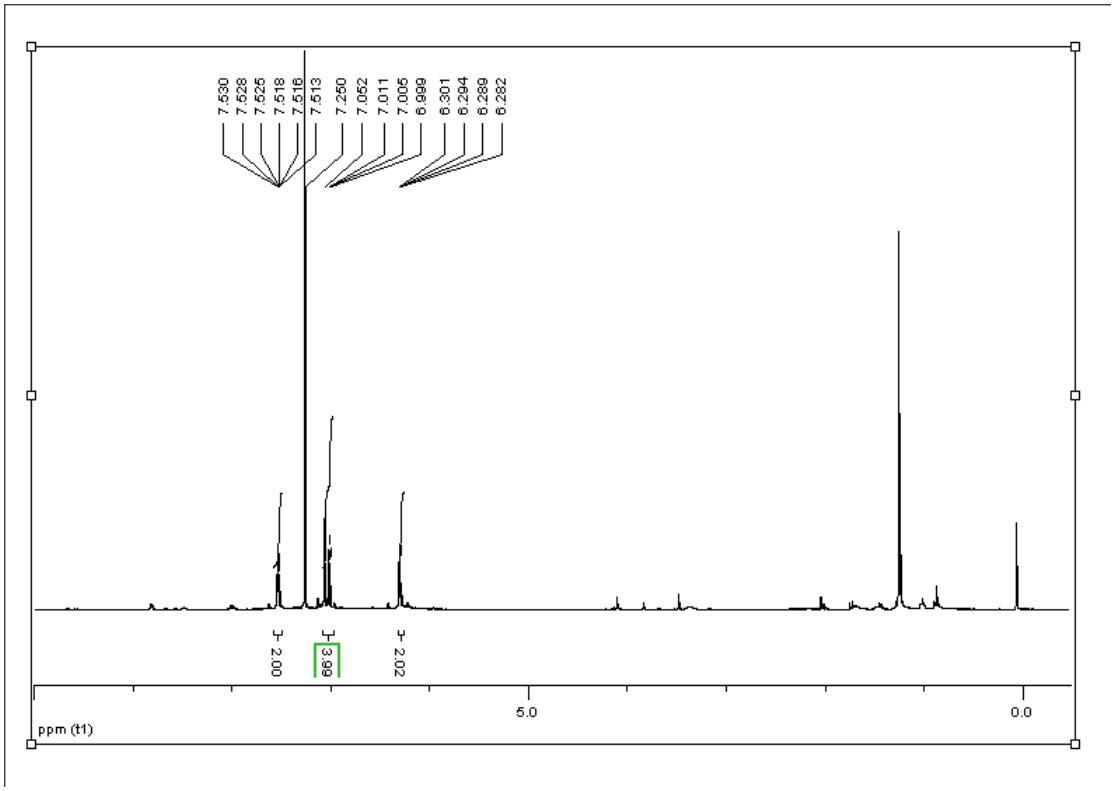


Initial product from reaction of thiophosgene with 1,1-di(pyrrol-1-yl)methane

^{1}H



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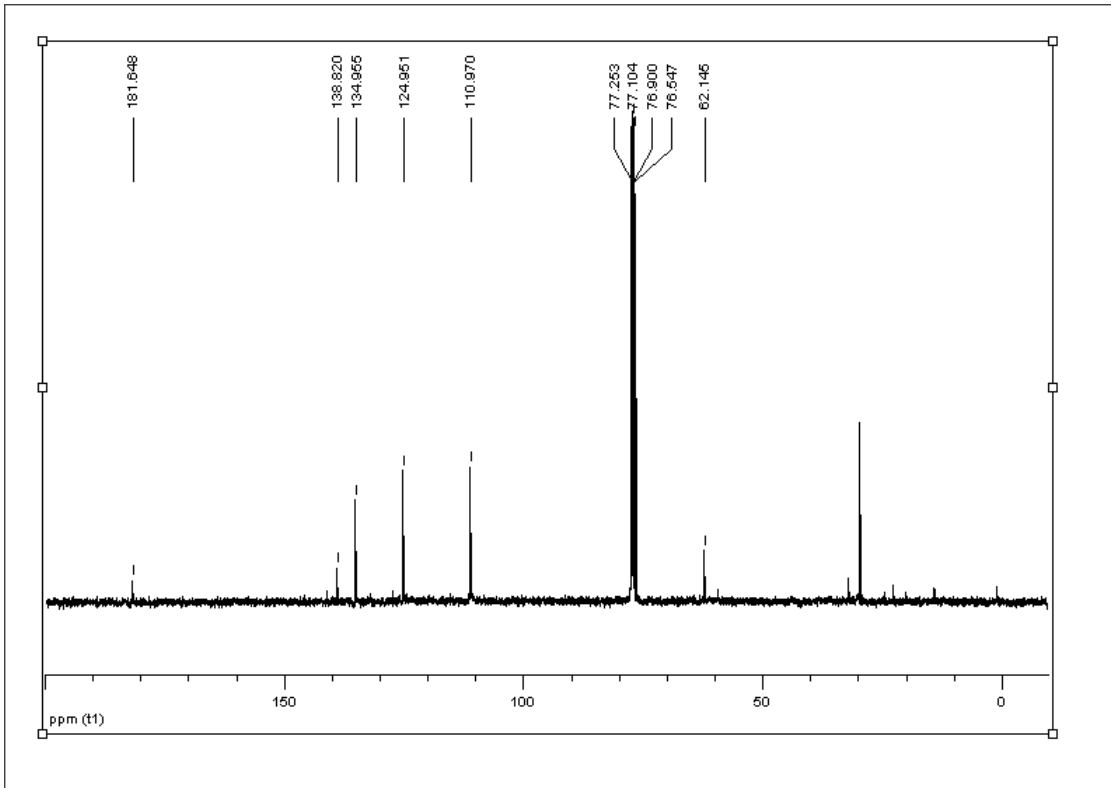

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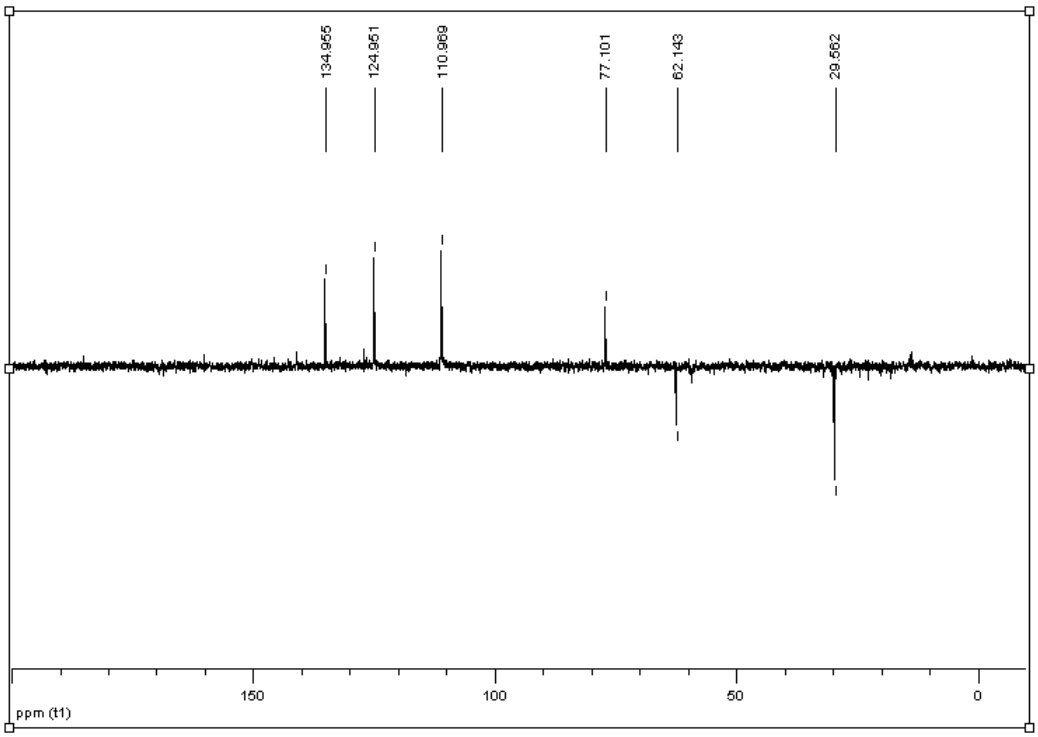

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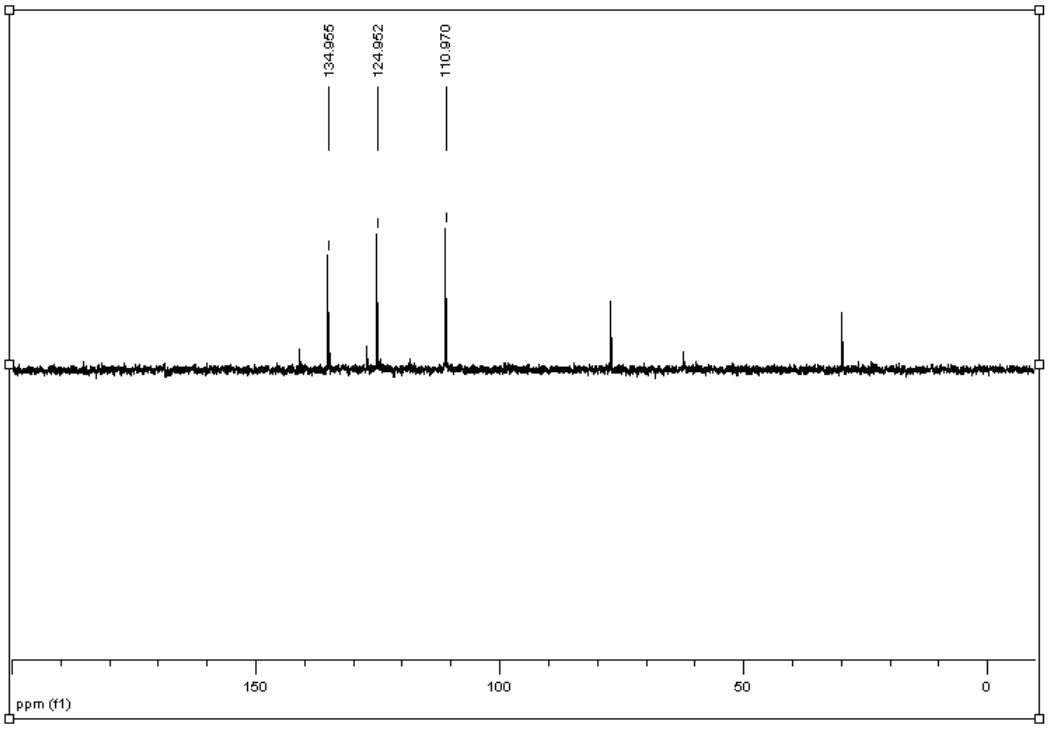
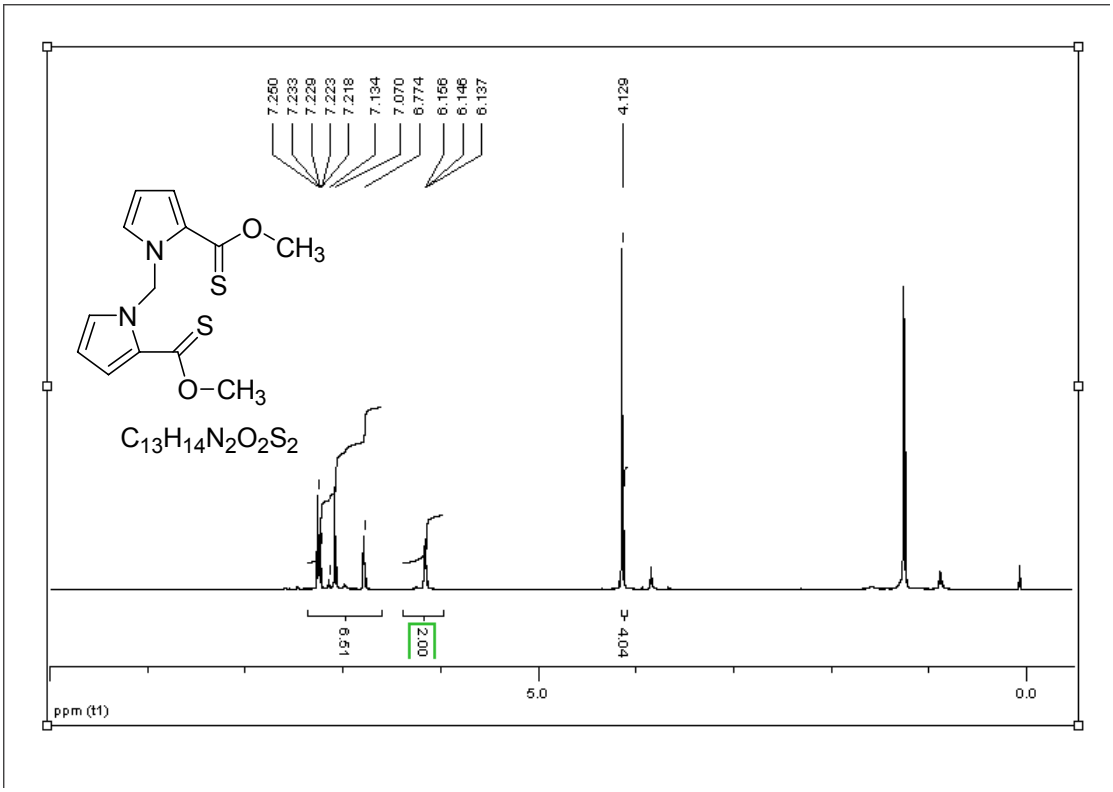


1,1-Di[2-(carbothiomethoxy)pyrrol-1-yl]methane 8

^{1}H



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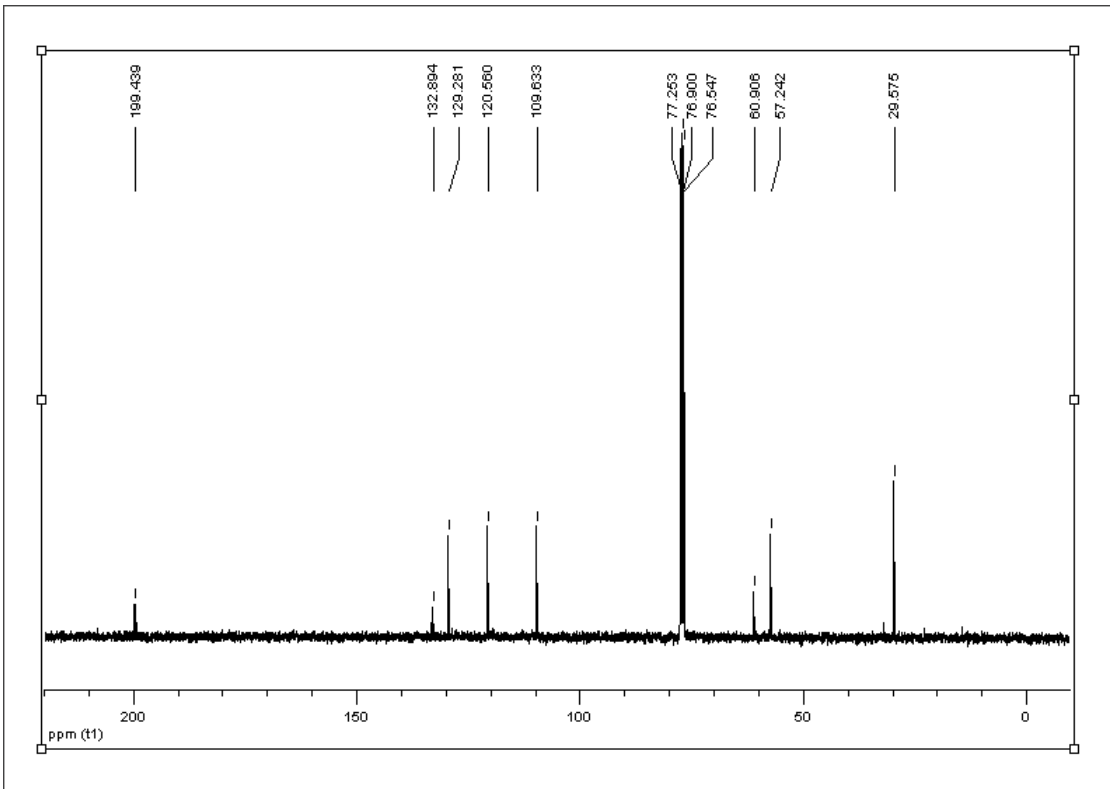

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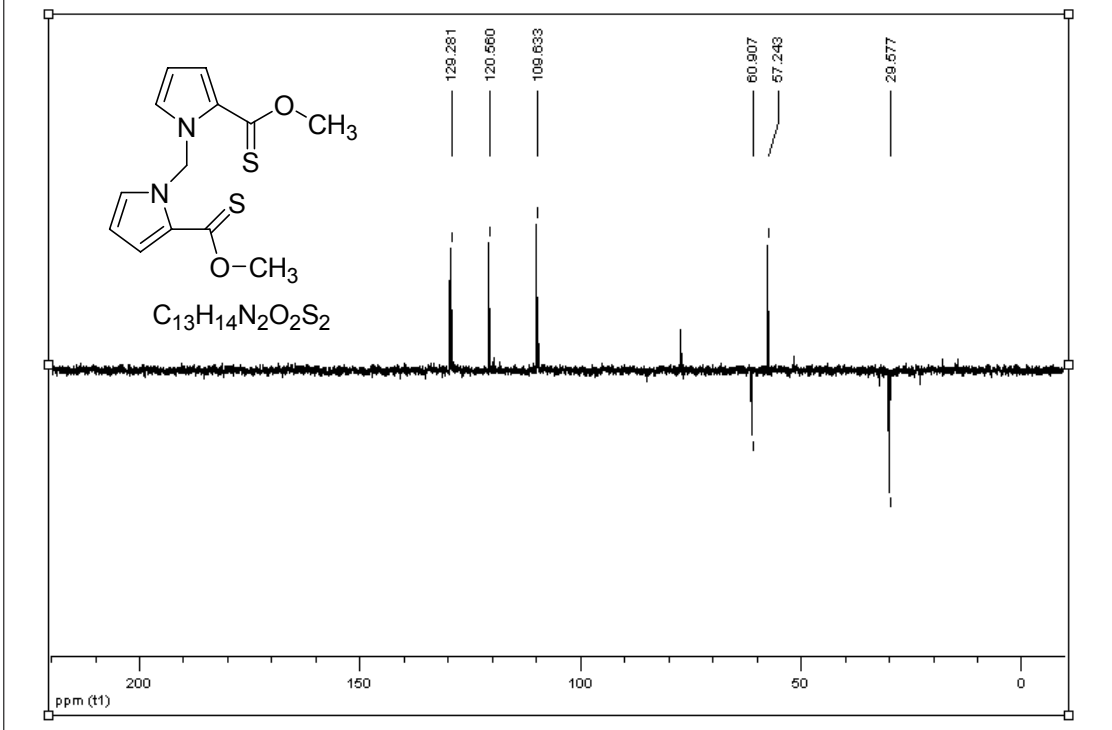

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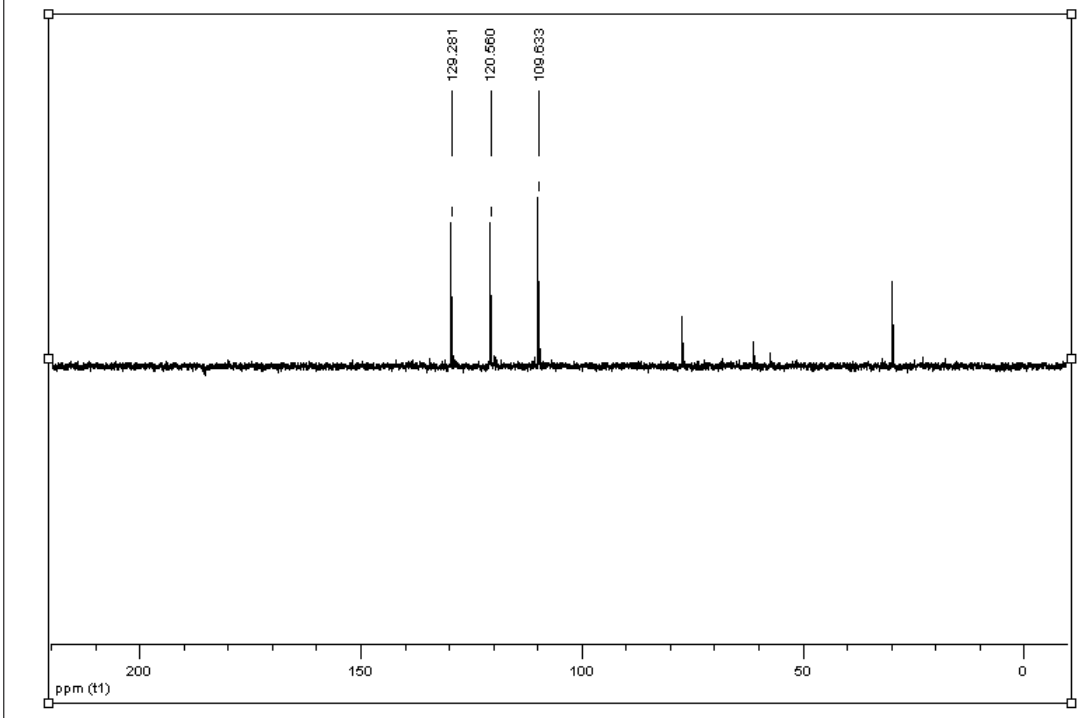
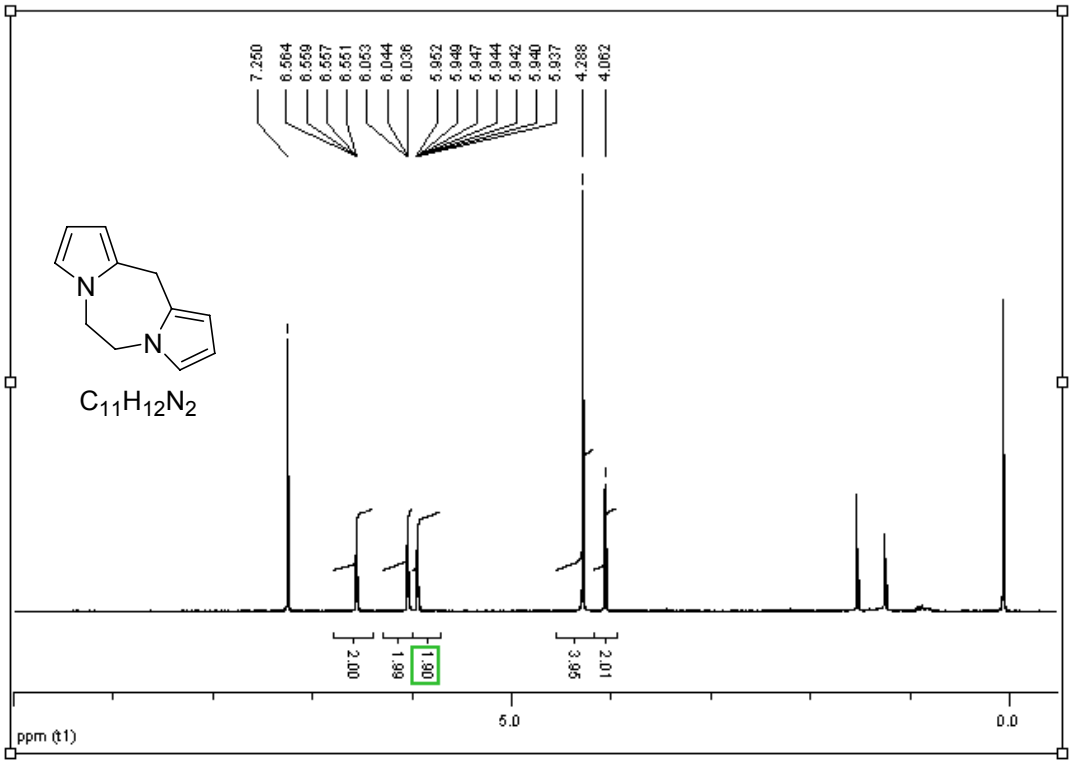


5,6-Dihydro-11*H*-dipyrrolo[1,2-*d*;2′,1′-*g*][1,4]diazepine 9

^{1}H



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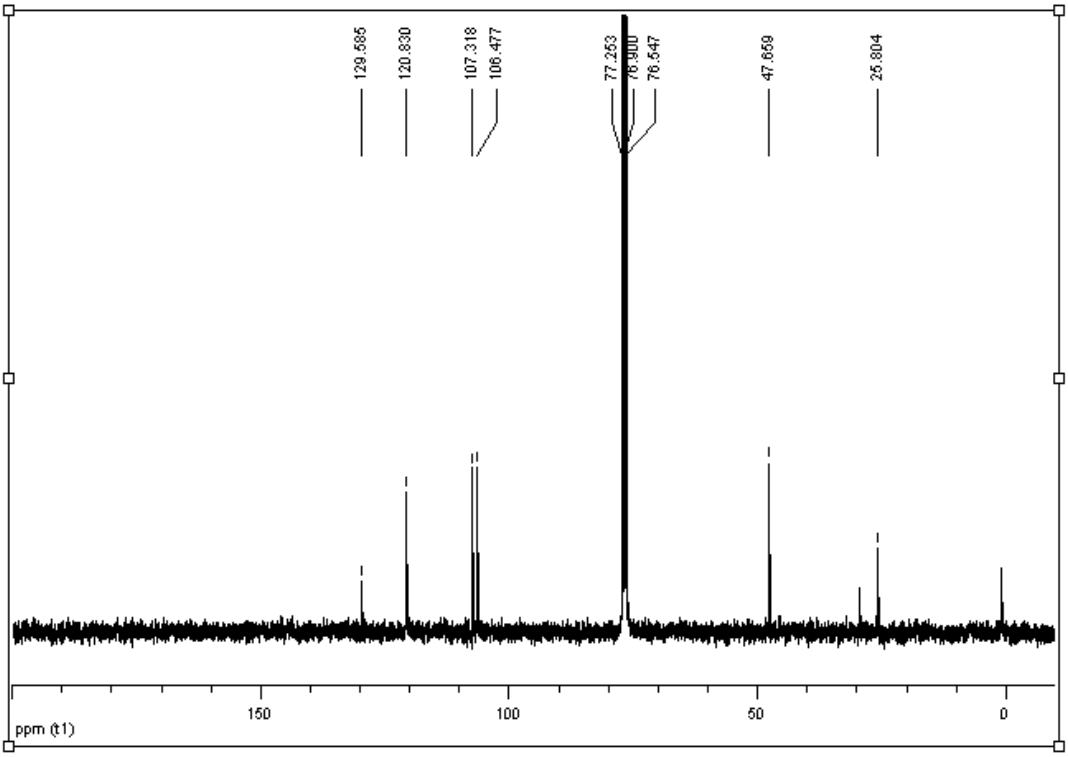

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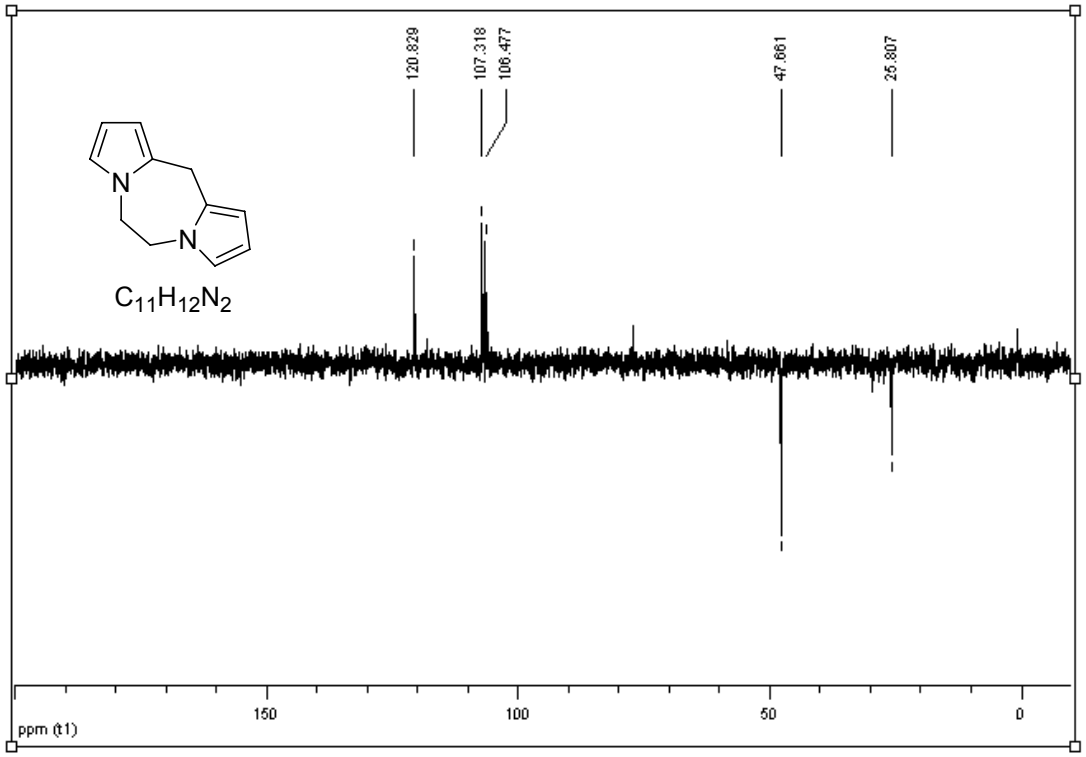

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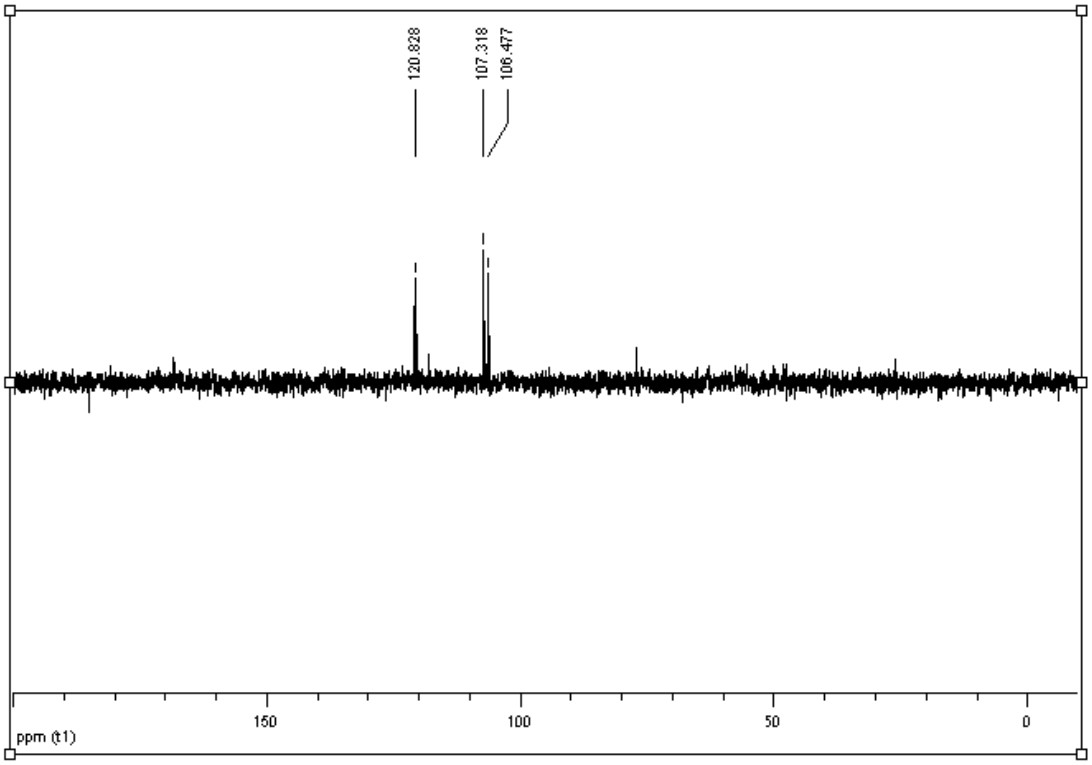
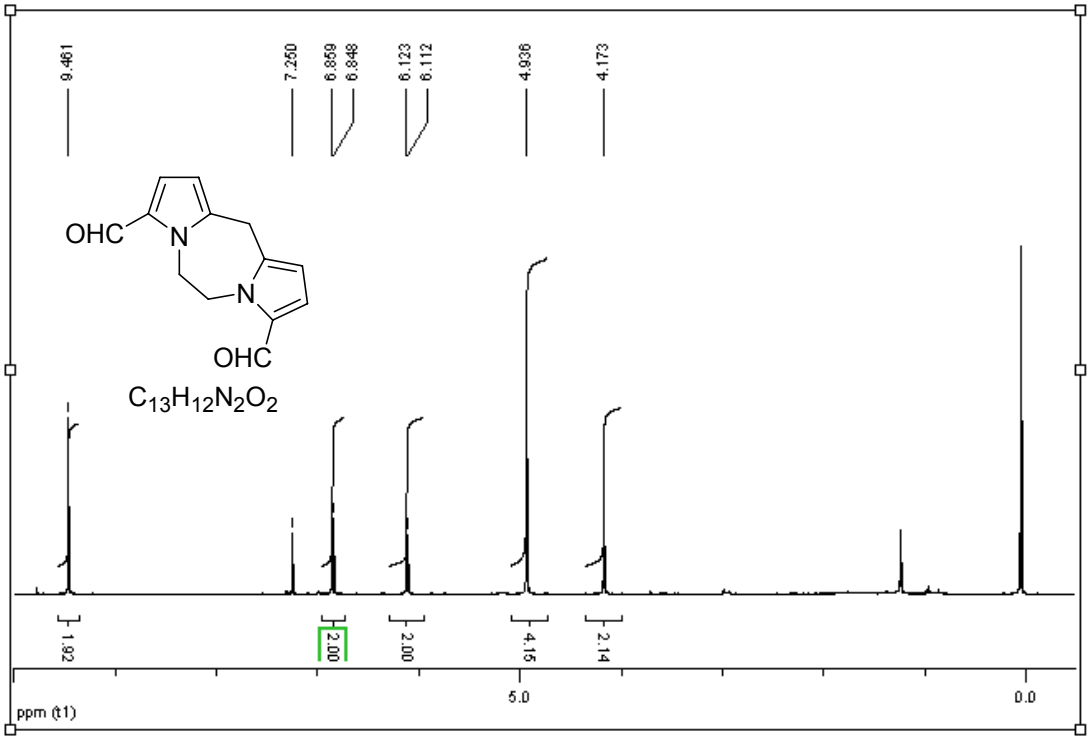


5,6-Dihydro-11*H*-dipyrrolo[1,2-*d*;2′,1′-*g*][1,4]diazepine-3,8-dicarbaldehyde 10

^{1}H



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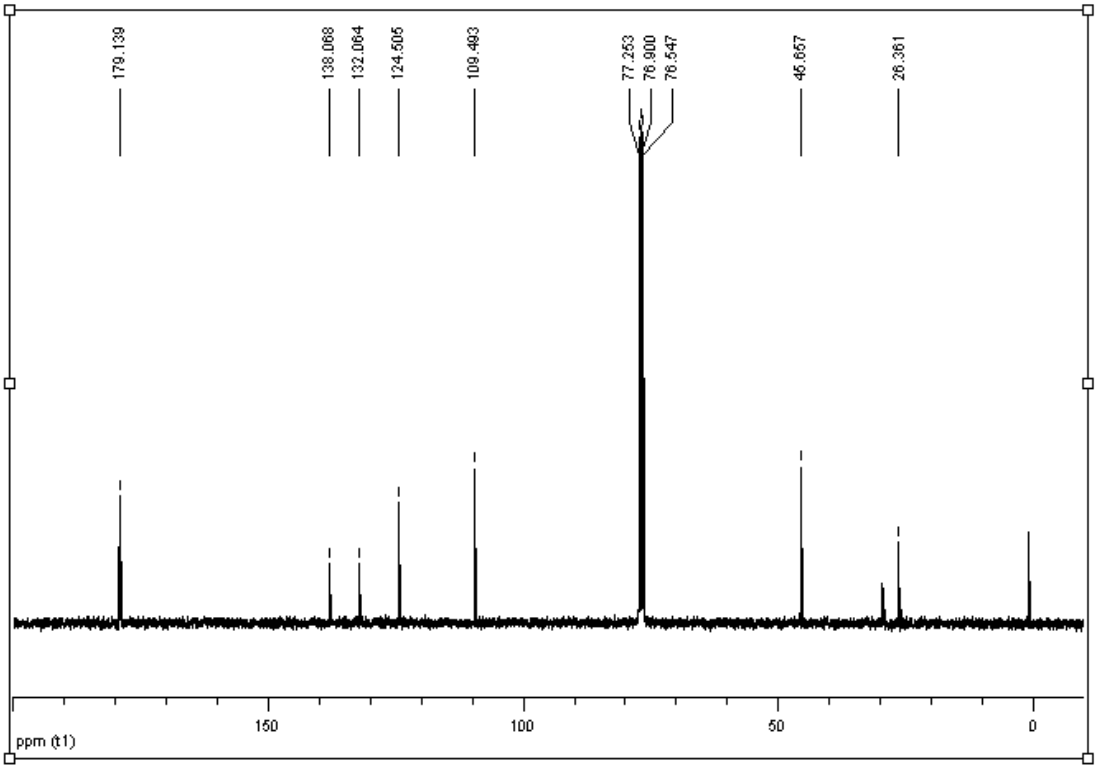

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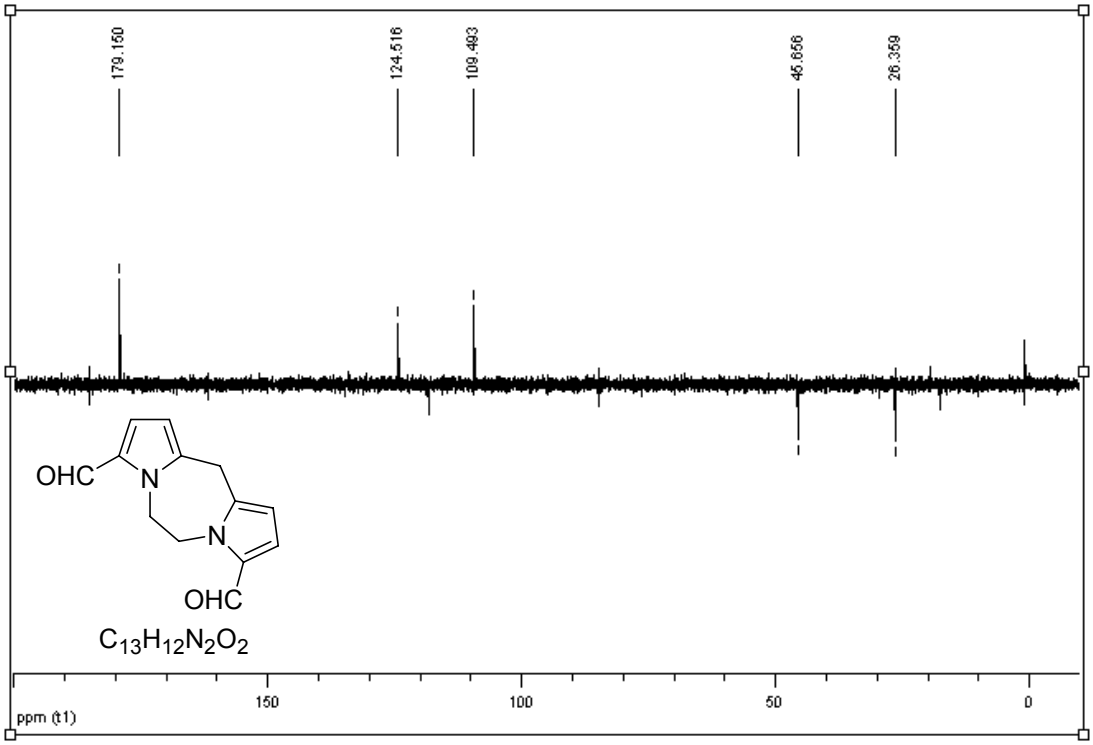

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