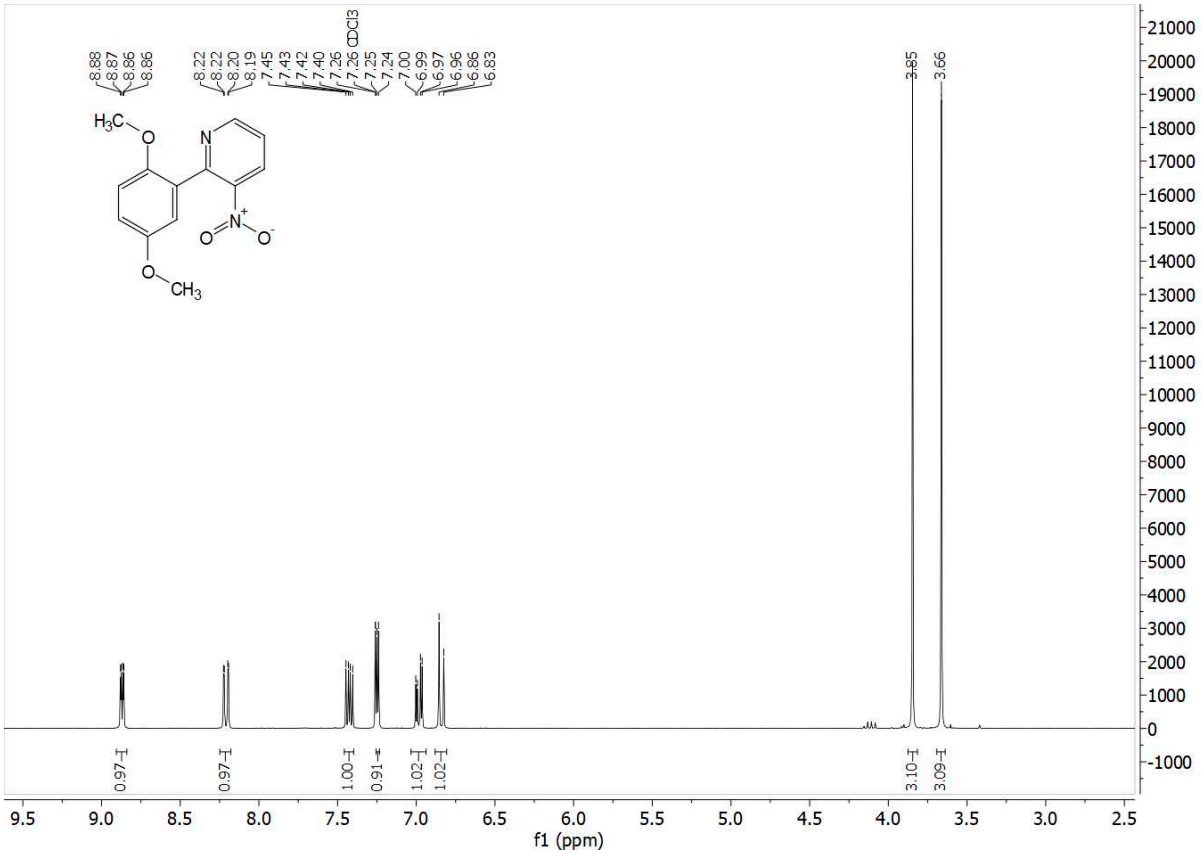
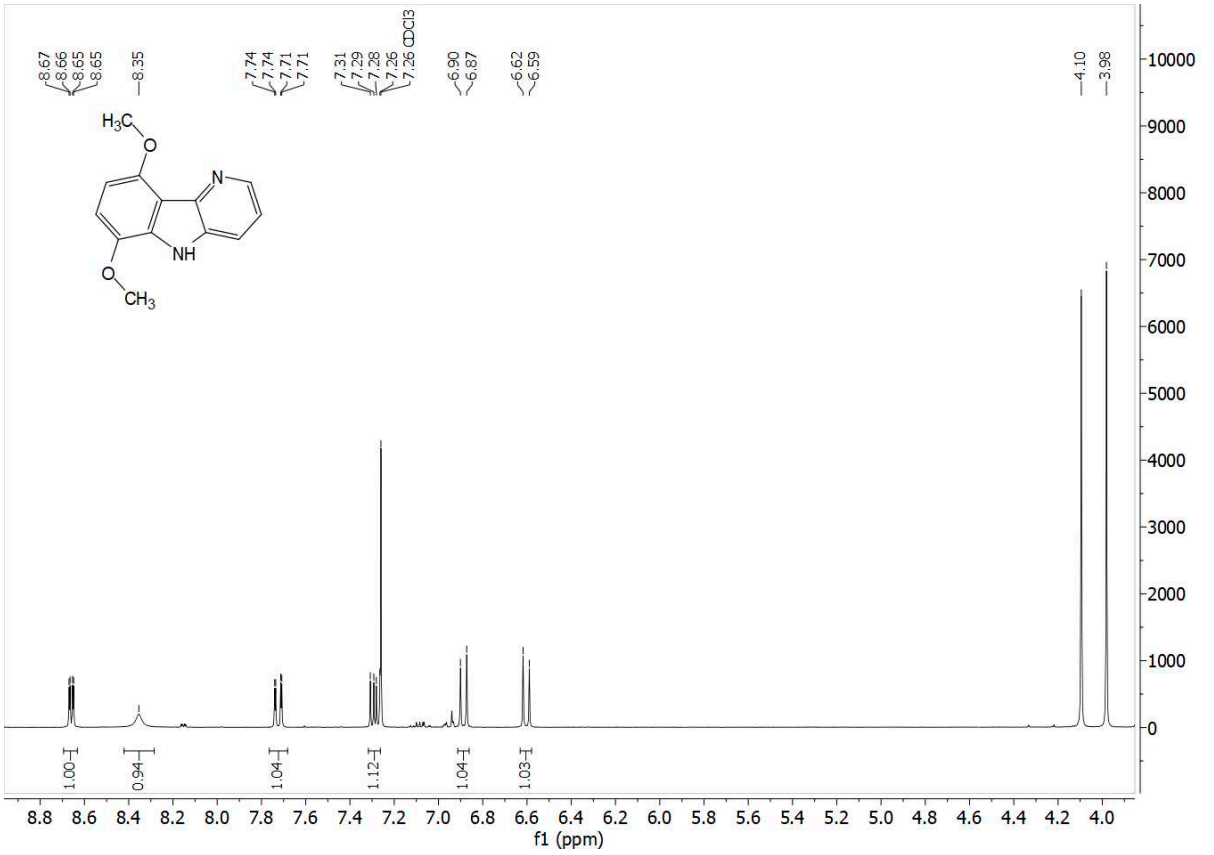
Supporting Material for:
2-(2,5-Dimethoxyphenyl)pyrrole-3-carbonitrile
By Yannic Grimm, Dieter Schollmeyer, Heiner Detert

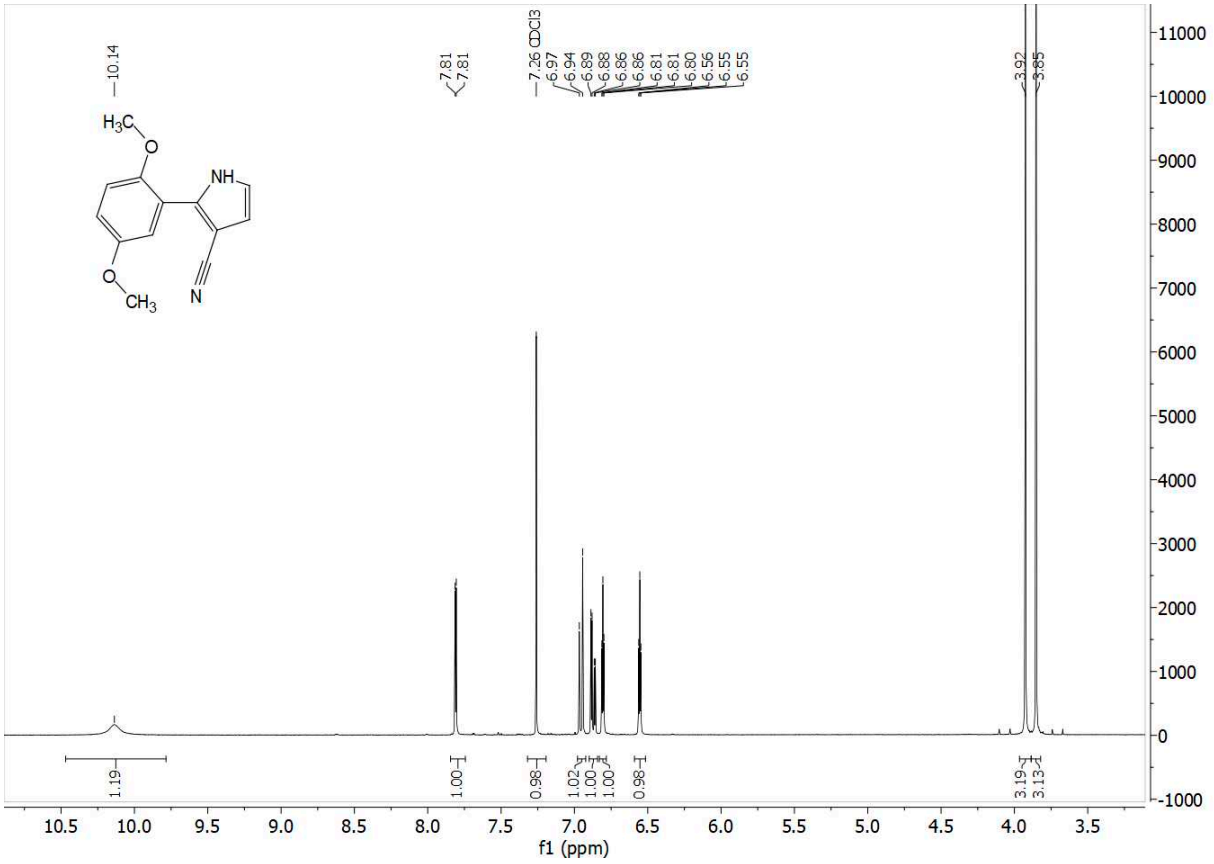
Content:



^{1}H-NMR Spectrium of 2-(2,5-dimethoxyphenyl)-3-nitropyridine

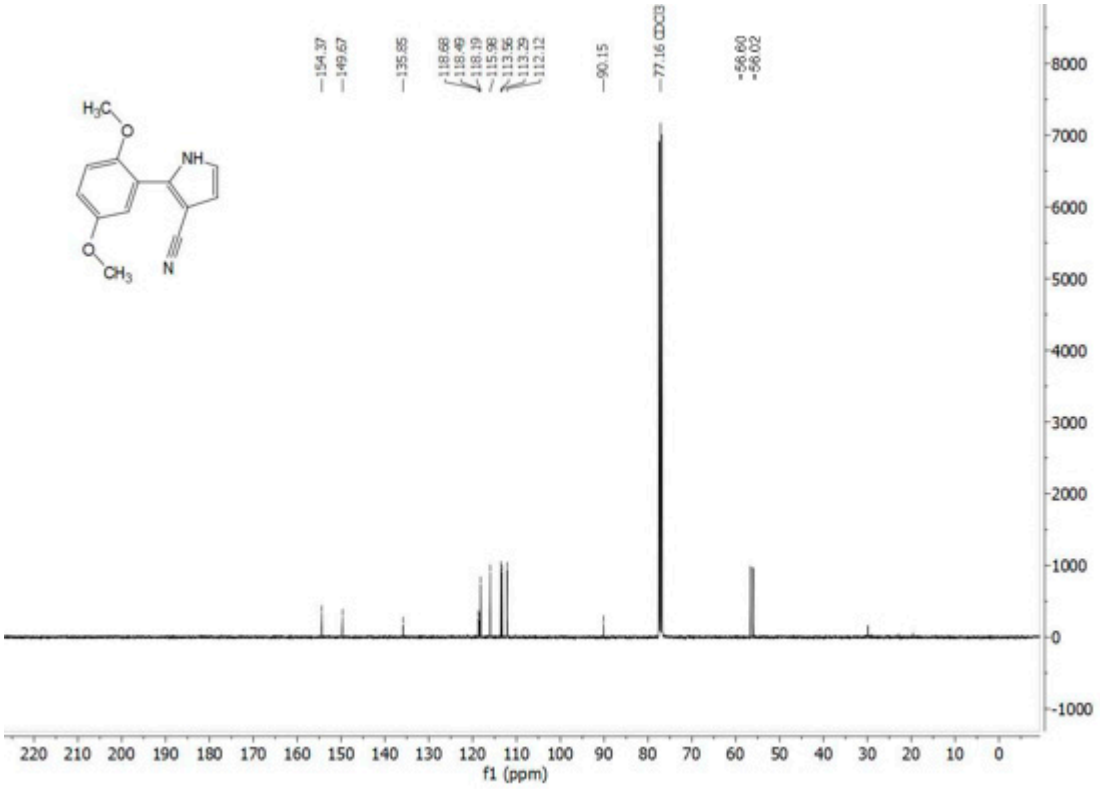


^{1}H-NMR Spectrum of dimethoxy-δ-carboline

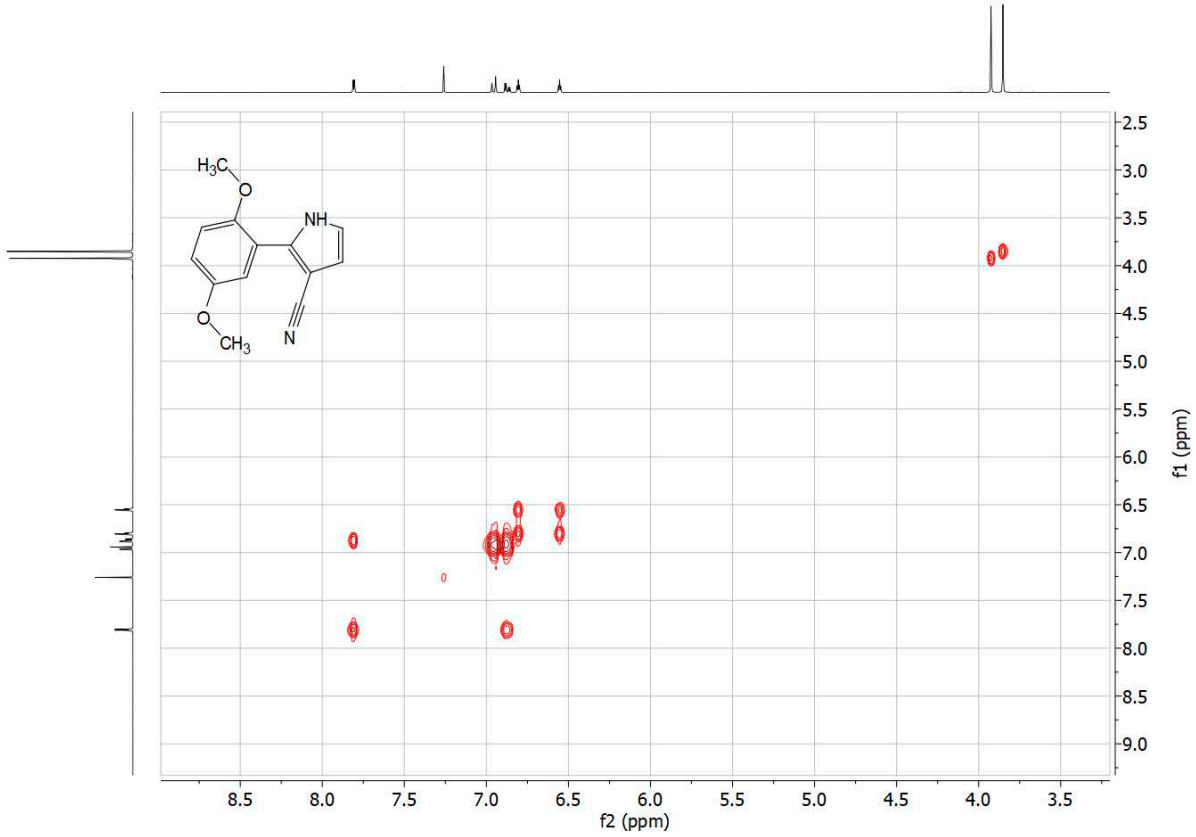


^{1}H-NMR Spectrum of 2-(2,5-dimethoxyphenyl)pyrrole-3-carbonitrile

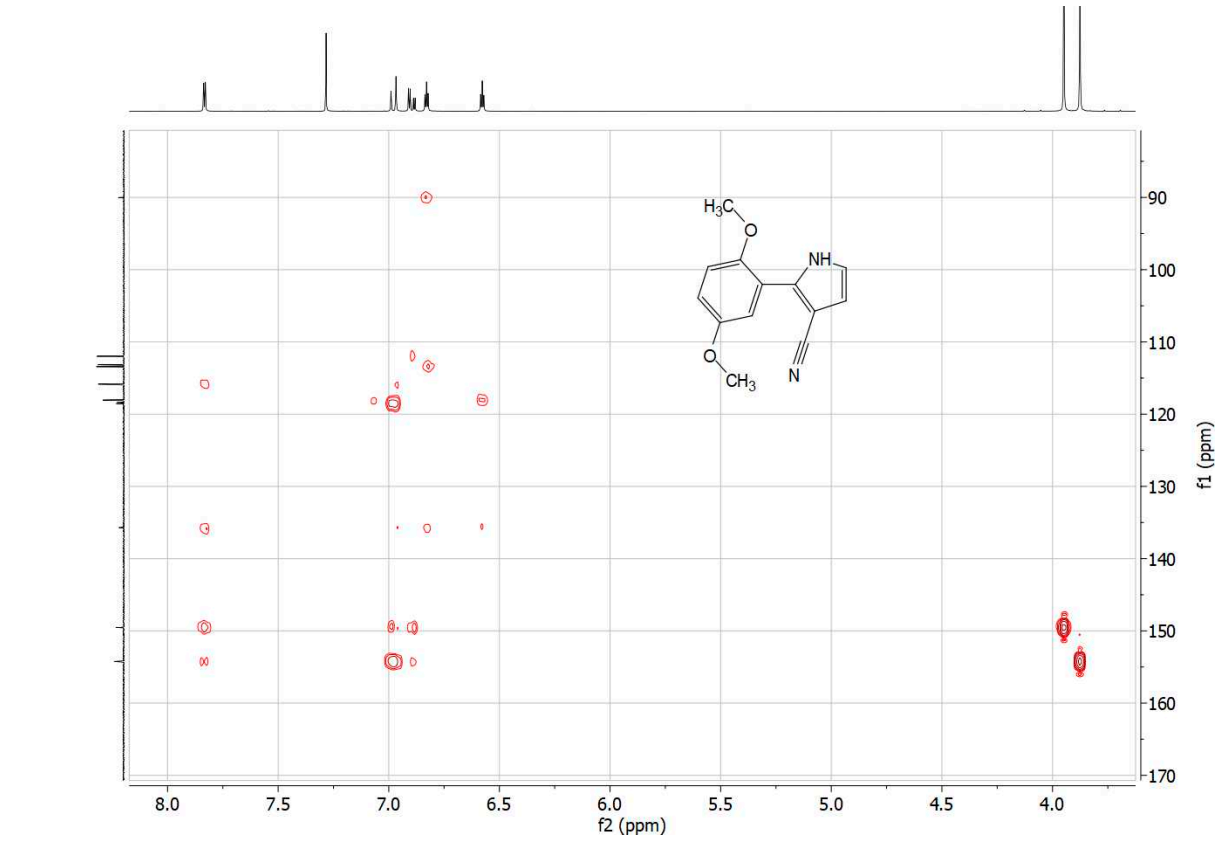
-56.60
-56.02



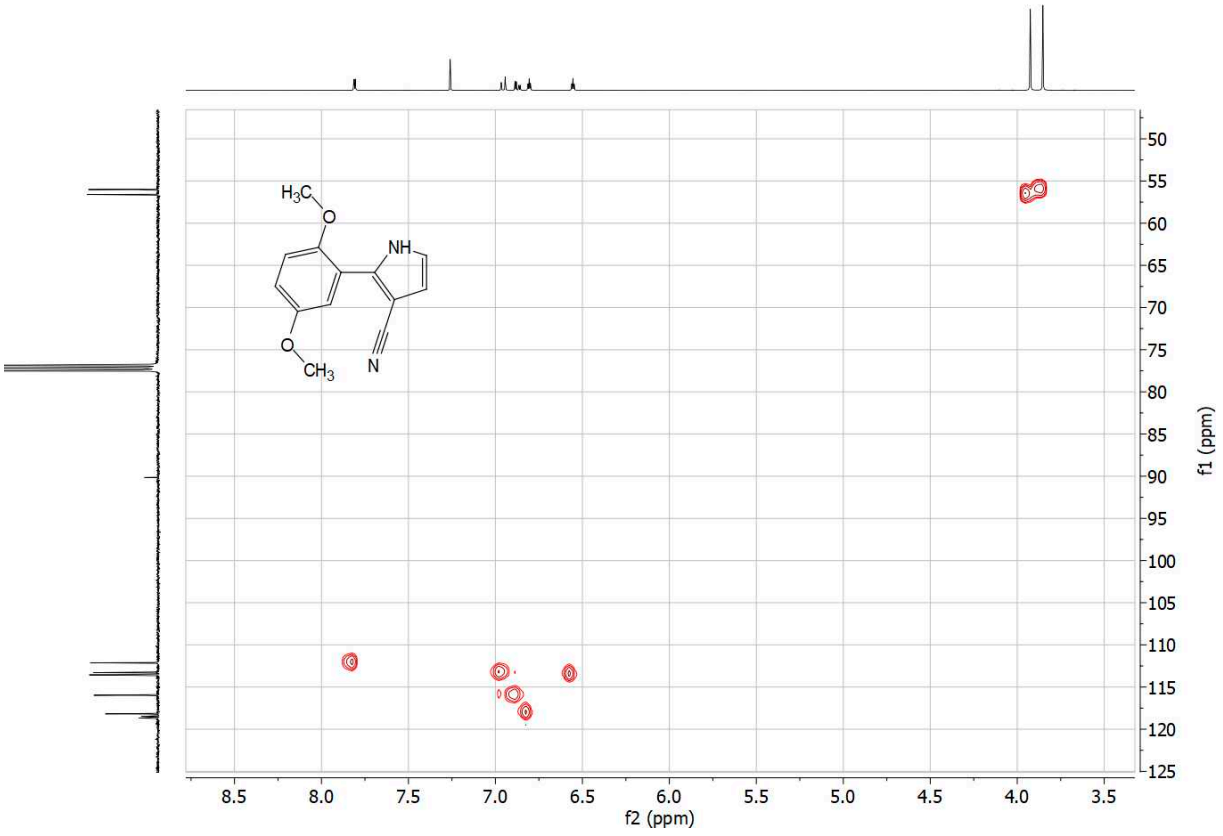
^{13}C-NMR Spectrum of 2-(2,5-dimethoxyphenyl)pyrrole-3-carbonitrile



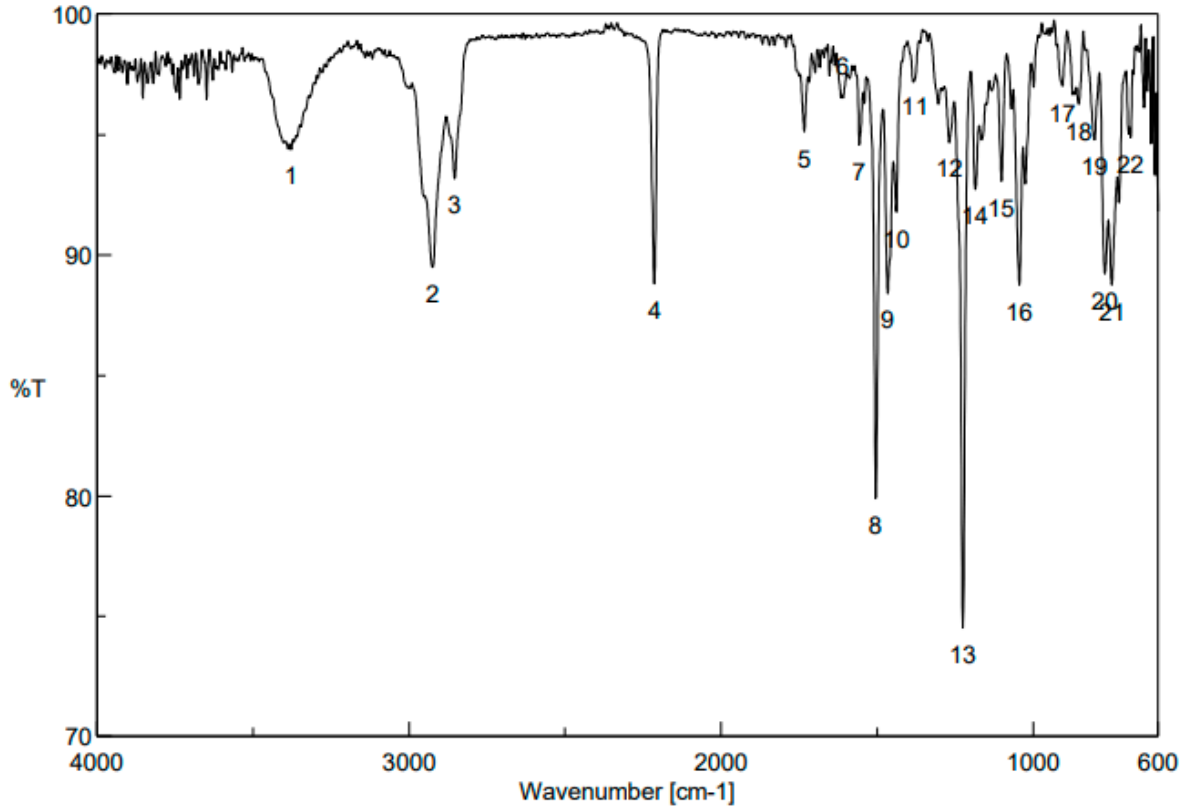
HH-COSY of 2-(2,5-dimethoxyphenyl)pyrrole-3-carbonitrile



HmbC of 2-(2,5-dimethoxyphenyl)pyrrole-3-carbonitrile



HSQC of 2-(2,5-dimethoxyphenyl)pyrrole-3-carbonitrile



Result of Peak Picking

No.	Position	Intensity	No.	Position	Intensity
1	3377.71	94.3718	2	2924.52	89.4877
3	2854.13	93.158	4	2213.88	88.8044
5	1733.69	95.1103	6	1612.2	96.6396
7	1557.24	94.547	8	1505.17	79.8722
9	1465.63	88.3854	10	1438.64	91.7779
11	1378.85	97.2821	12	1267.97	94.6749
13	1224.58	74.5007	14	1186.01	92.7194
15	1102.12	93.0626	16	1044.26	88.7511
17	905.415	96.9904	18	853.347	96.238
19	803.206	94.7639	20	770.423	89.2133
21	748.245	88.7614	22	687.498	94.863

[Comment]

Sample Name	
Comment	
User	
Division	
Company	Johannes Gutenberg - Universität

[Measurement Information]

Model Name	FT/IR-4100typeA
Serial Number	B070161016
Light Source	Standard
Detector	TGS
Accumulation	16
Resolution	4 cm-1
Zero Filling	On
Apodization	Cosine
Gain	Auto (128)
Aperture	Auto (7.1 mm)
Scanning Speed	Auto (2 mm/sec)
Filter	Auto (30000 Hz)

IR-Spectrum (ATR, neat) of 2-(2,5-Dimethoxyphenyl)pyrrole-3-carbonitrile

X-ray crystallography data		
CCDC number	2247185	
Empirical formula	$C_{13}H_{12}N_2O_2$	
moiety formula	$C_{13}H_{12}N_2O_2$	
Formula weight	228.25	
Temperature	193(2) K	
Wavelength, radiation type	0.71073Å, MoKα	
Diffractometer	STOE IPDS 2T	
Crystal system	Monoclinic	
Space group name, number	C 2/c, (15)	
Unit cell dimensions	a = 21.8244(9) Å	α = 90°
	b = 21.8779(9) Å	β = 114.583(3)°
	c = 21.0043(9) Å	γ = 90°
Volume	9119.9(7) $Å^3$	
Number of reflections	10685	
and range used for lattice parameters	2.65° <=θ<= 28.44°	
Z	32	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.9880 and 0.9338	
F(000)	3840	
Crystal size, colour and form	0.120 x 0.240 x 0.850 mm^3, colorless needle	
Theta range for data collection	2.145 to 28.364°.	
Index ranges	-29<=h<=29, -26<=k<=29, -27<=l<=27	
Number of reflections:		
collected	29739	
independent	11283 [R(int) = 0.0928]	
observed [I>2sigma(I)]	5857	
Completeness to theta = 25.2°	99.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11283 / 0 / 789	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0623, wR2 = 0.1458	
R indices (all data)	R1 = 0.1309, wR2 = 0.1799	
Largest diff. peak and hole	0.237 and -0.320 $eÅ^{-3}$	