Supporting Information

***Rec. Nat. Prod*. 14:2 (2020) 98-104**

A New 2,*2′*-dipyridine and Its Congeners from Endophytic *Streptomyces* sp. KIB H017c with Potent Cytotoxicity

Xiao-Yan Ma[1,2], Feng-Xian Yang[2,3] and Sheng-Xiong Huang[*1,2]

[1] School of Chemical Engineering, Sichuan University of Science & Engineering, Zigong, 643000, PR China

[2] State Key Laboratory of Phytochemistry and Plant Resources in West China, CAS Center for Excellence in Molecular Plant Sciences, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204, China

[3]University of the Chinese Academy of Sciences, Beijing 100049, China

Table of contents	Page

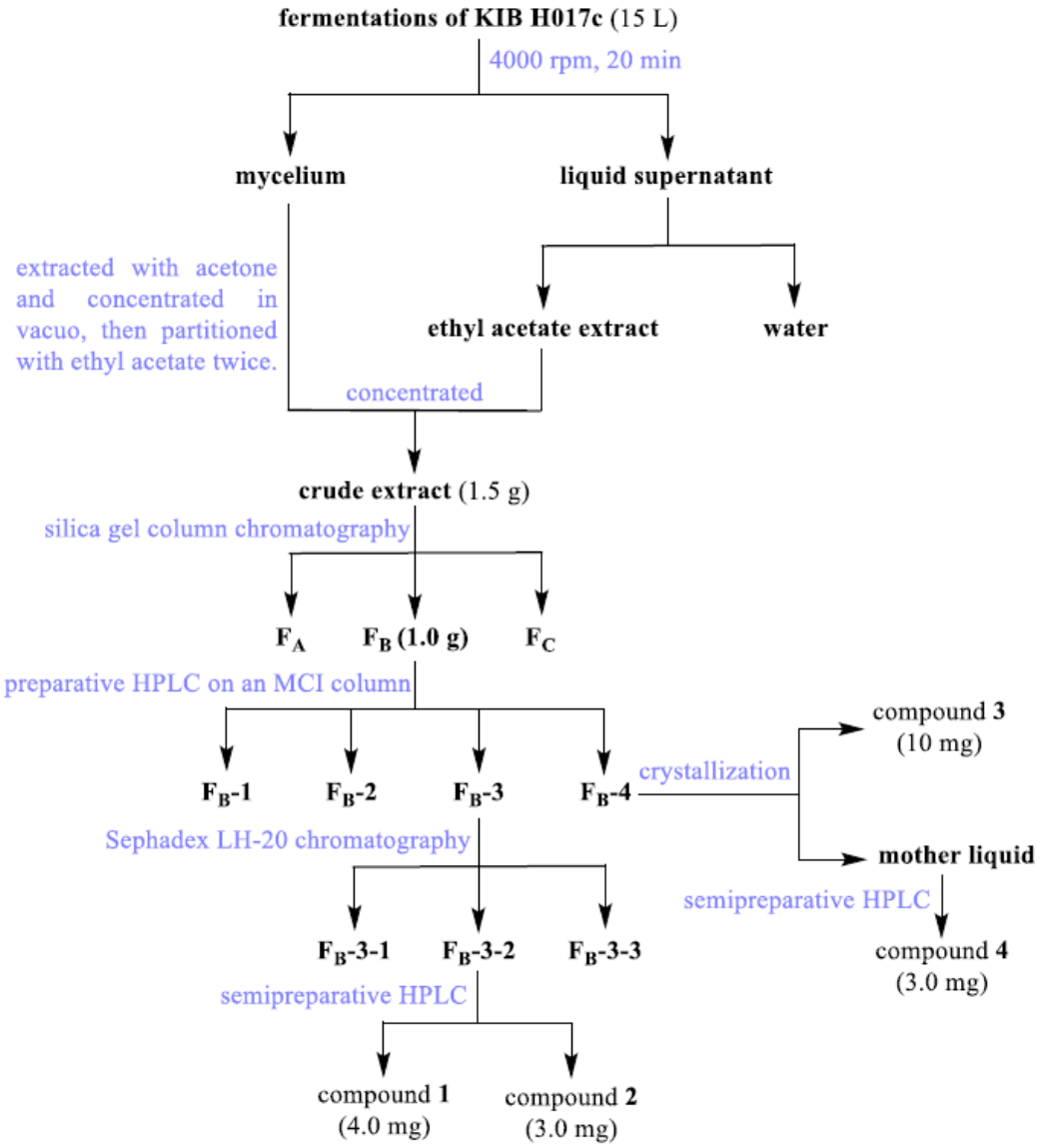


Figure S1: The separation scheme of KIB H017c

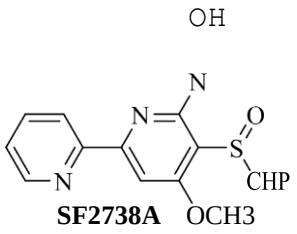


Figure S2: The structure of SF2738A

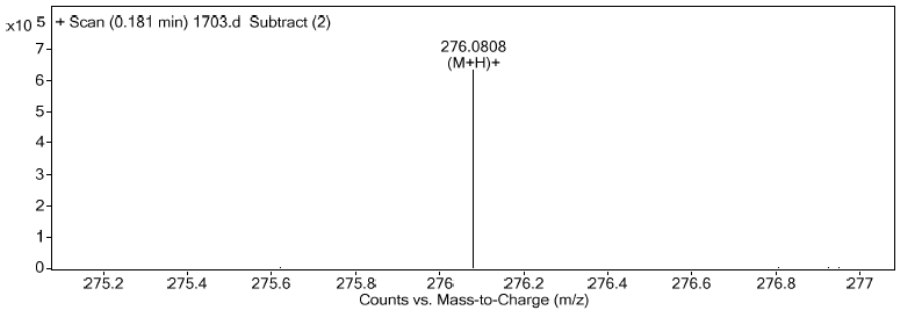
Qualitative Analysis Report

Data Filename	1703.d	**Sample Name**	1703
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	1/11/2016 10:43:09 AM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
276.0808	1	635276.19	C13 H13 N3 O2 S	(M+H)+
277.0831	1	94174.94	C13 H13 N3 O2 S	(M+H)+
278.0786	1	27269.65	C13 H13 N3 O2 S	(M+H)+
298.0625	1	680455.75		
299.0654	1	93391.07		
300.0603	1	30508.81		
314.036	1	76110.13		
573.1344	1	61809.84		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
S	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C13 H13 N3 O2 S	275.0729	276.0801	276.0808	-0.6	-2.1	9.0000

Figure S3: HRESI-MS spectrum of compound **1**

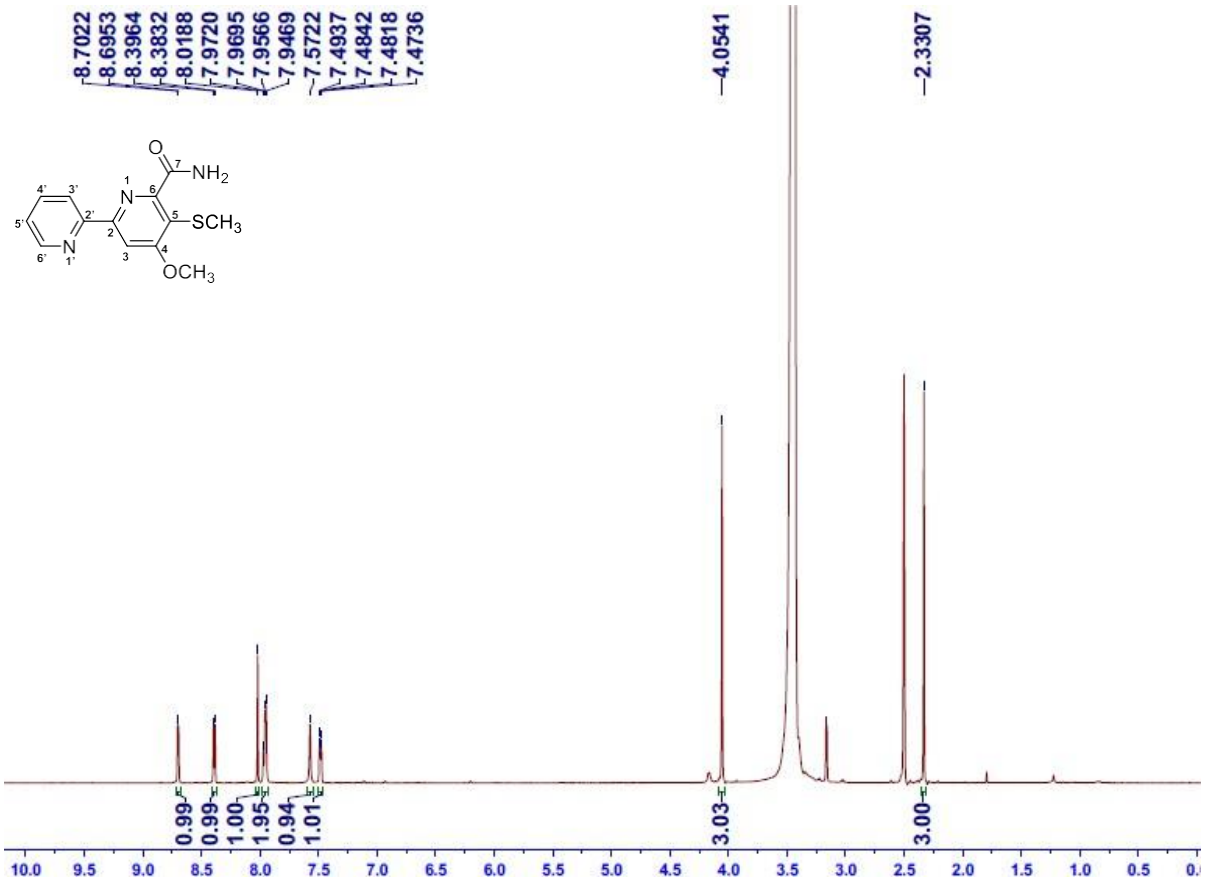


Figure S4: ^{1}H NMR spectrum of compound **1** (in DMSO-d_6, 600 MHz)

^{1}H NMR (DMSO-d_6, 600 MHz), δ: 2.33 (3H, s, 5-SCH_3), 4.05 (3H, s, 4-OCH_3), 7.48 (1H, ddd, J = 7.2, 4.8, 1.2 Hz), 7.57 (1H,s, 7-NH), 7.94 (1H, m, 7-NH), 7.96 (1H, (1H, td, J = 7.8, 1.2 Hz, H-4'), 8.02 (1H, s, H-3), 8.39 (1H, d, J = 7.8 Hz, H-3'), 8.70 (1H, d, J = 4.2 Hz, H-6').

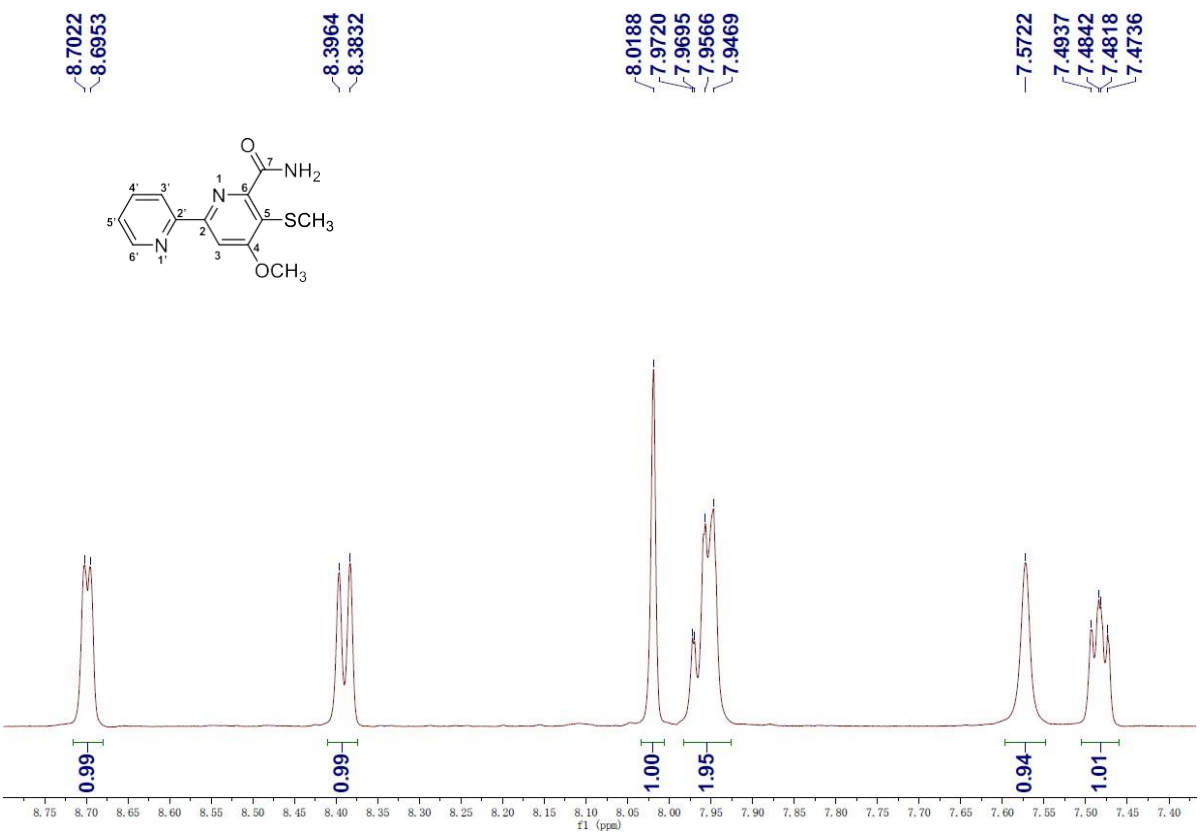


Figure S5: ^{1}H NMR spectrum of compound **1** (From 7.40 to 8.75 ppm)

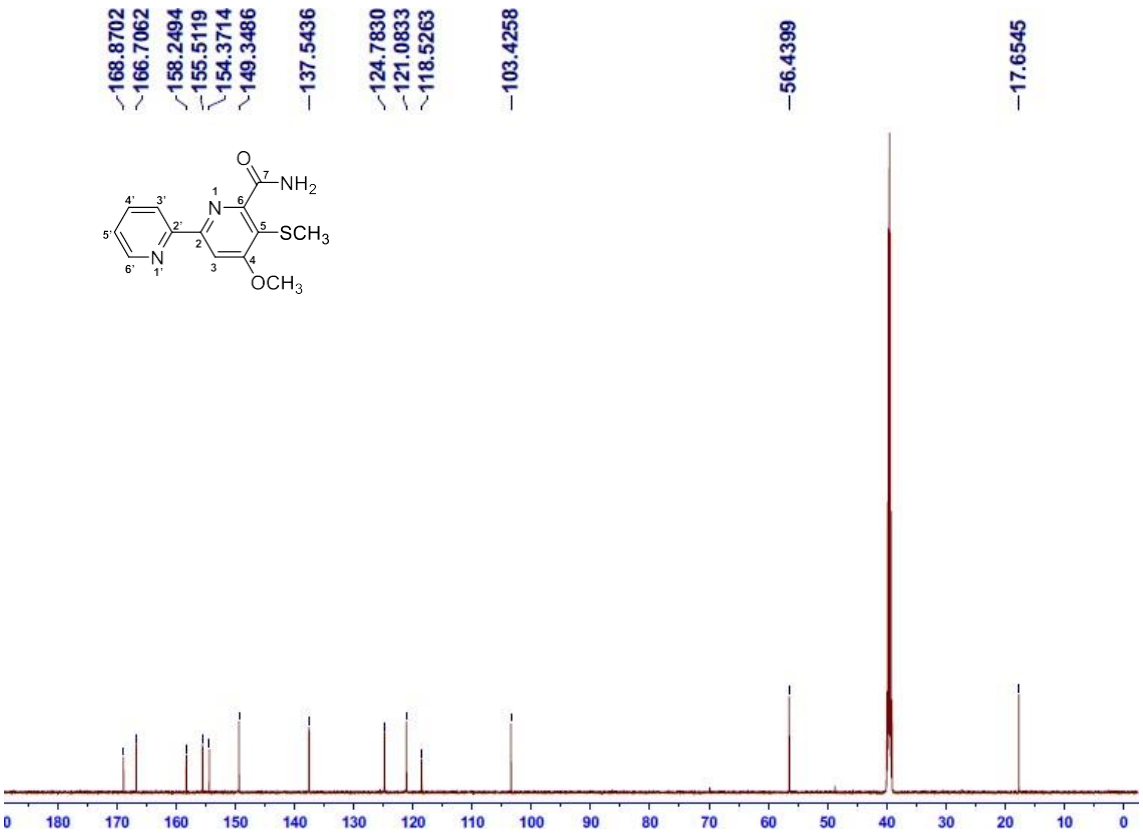


Figure S6: ^{13}C NMR spectrum of compound **1** (in DMSO-d_6, 150 MHz)

^{13}C NMR (DMSO-d_6, 150 MHz), δ 168.9 (C-6), 166.7 (C-4), 158.2 (C-5), 155.5 (C-2), 154.4 (C-2′), 149.3 (CH-6′), 137.5 (CH-4′), 124.8 (CH-5′), 121.1 (CH-3′), 118.5 (C-5), 103.4 (CH-3), 56.4 (C-[4-OCH_3]), 17.6 (C-[5-SCH_3]).

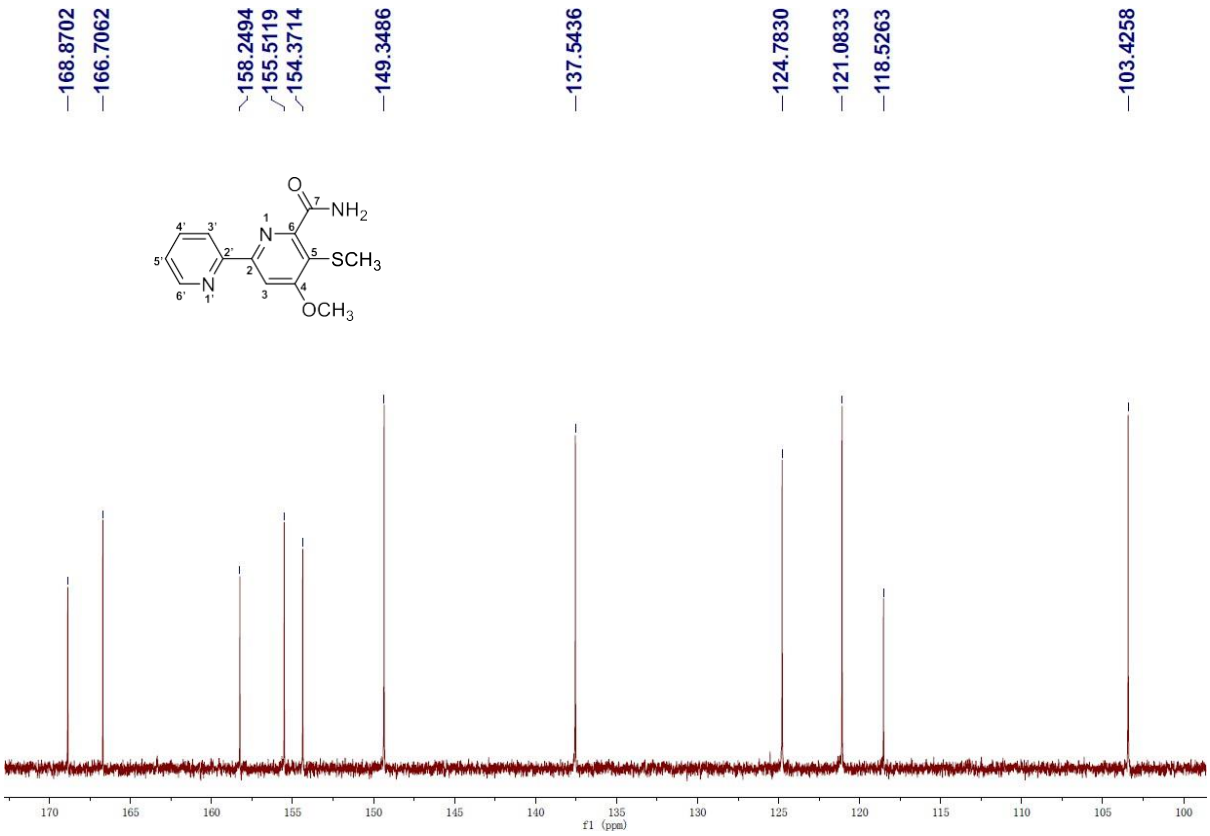


Figure S7: ^{13}C NMR spectrum of compound **1** (From 100 to 170 ppm)

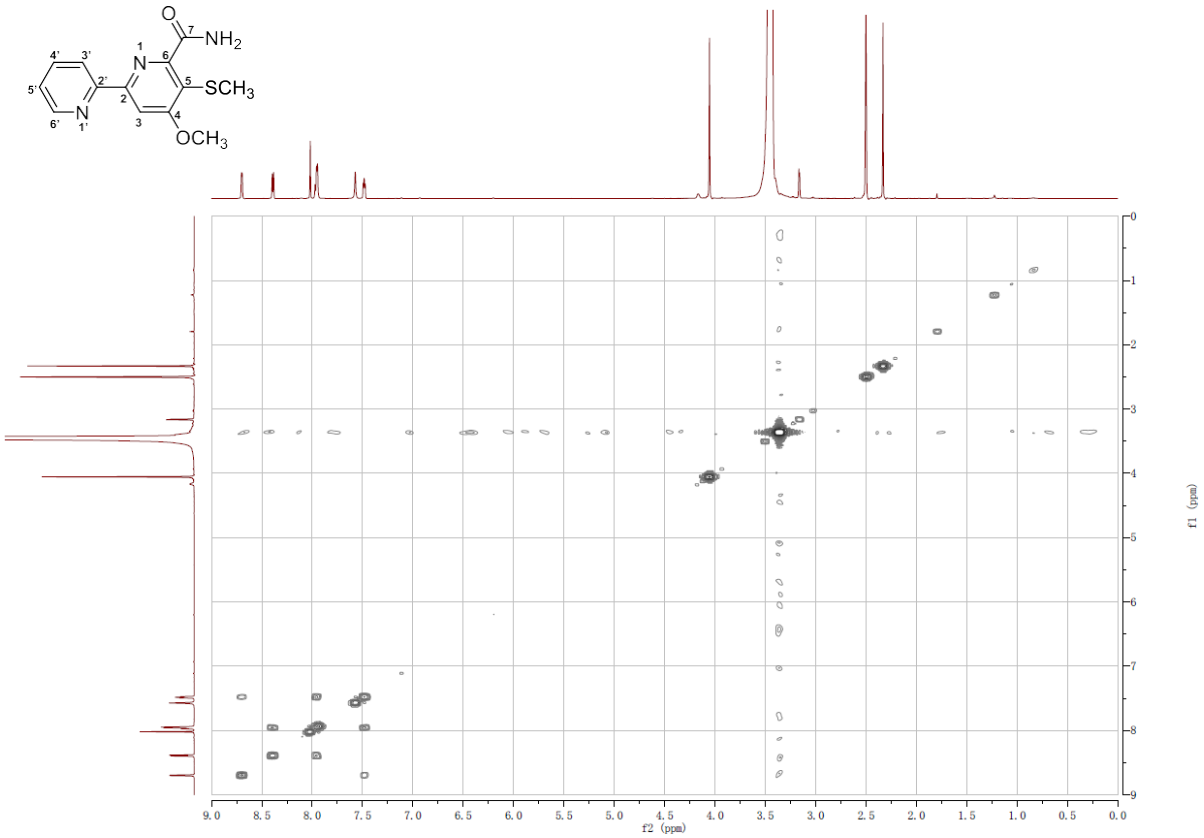


Figure S8: H-H COSY spectrum of compound **1** (in DMSO-d_6)

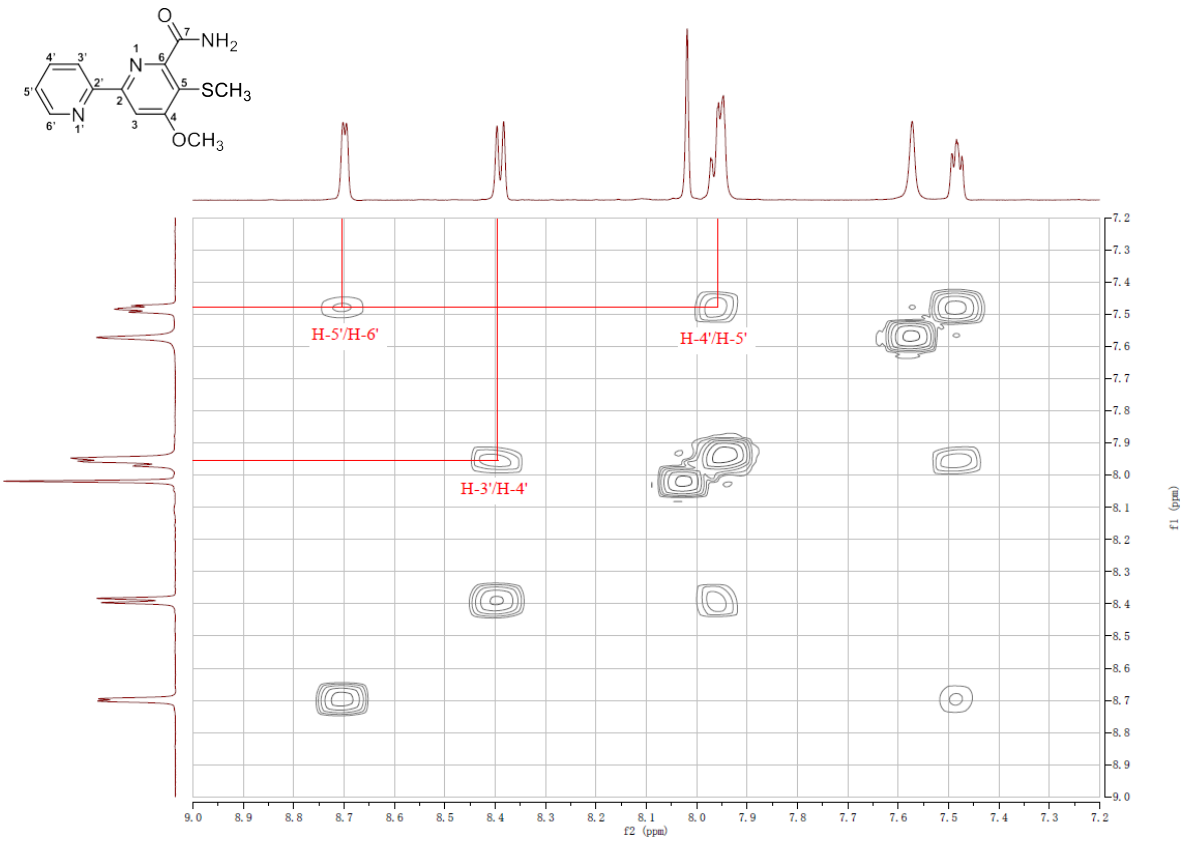


Figure S9: H-H COSY spectrum of compound **1** (From 7.20 to 9.00 ppm）

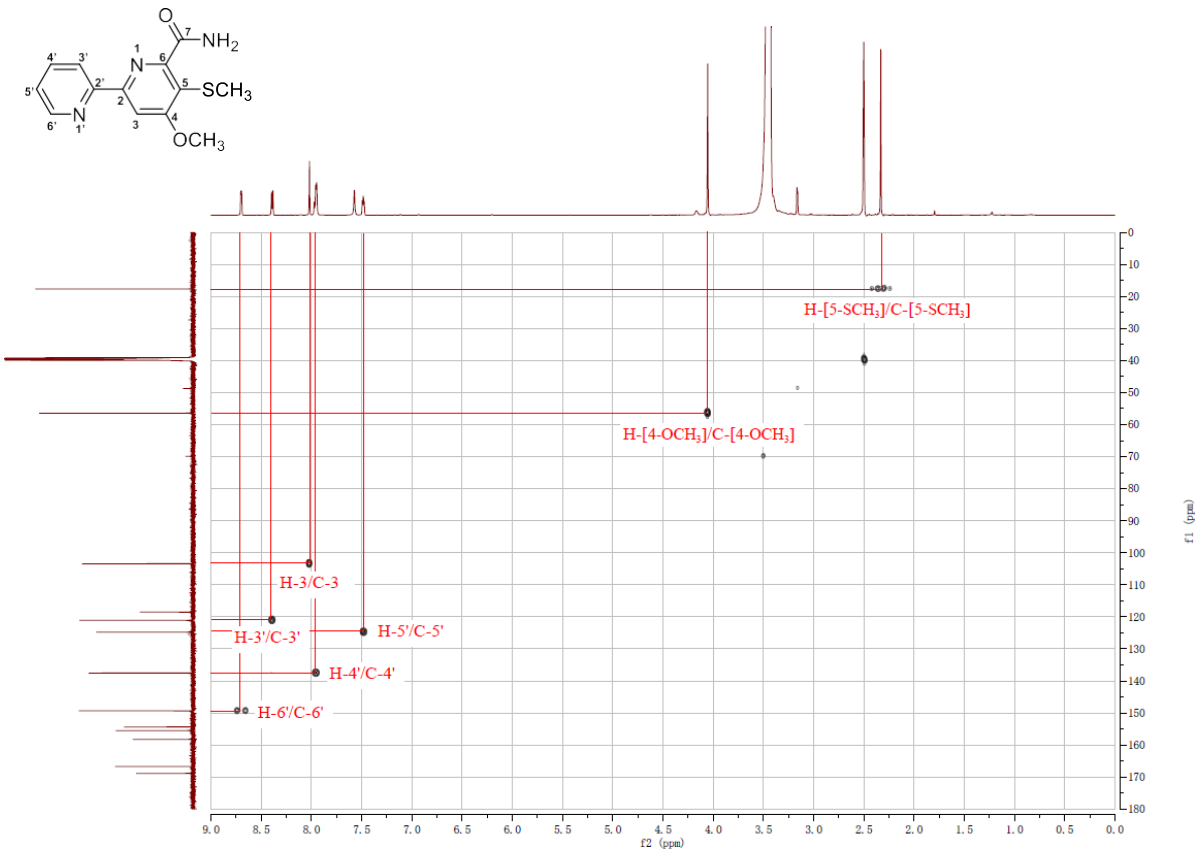


Figure S10: HSQC spectrum of compound **1** (in DMSO-d_6)

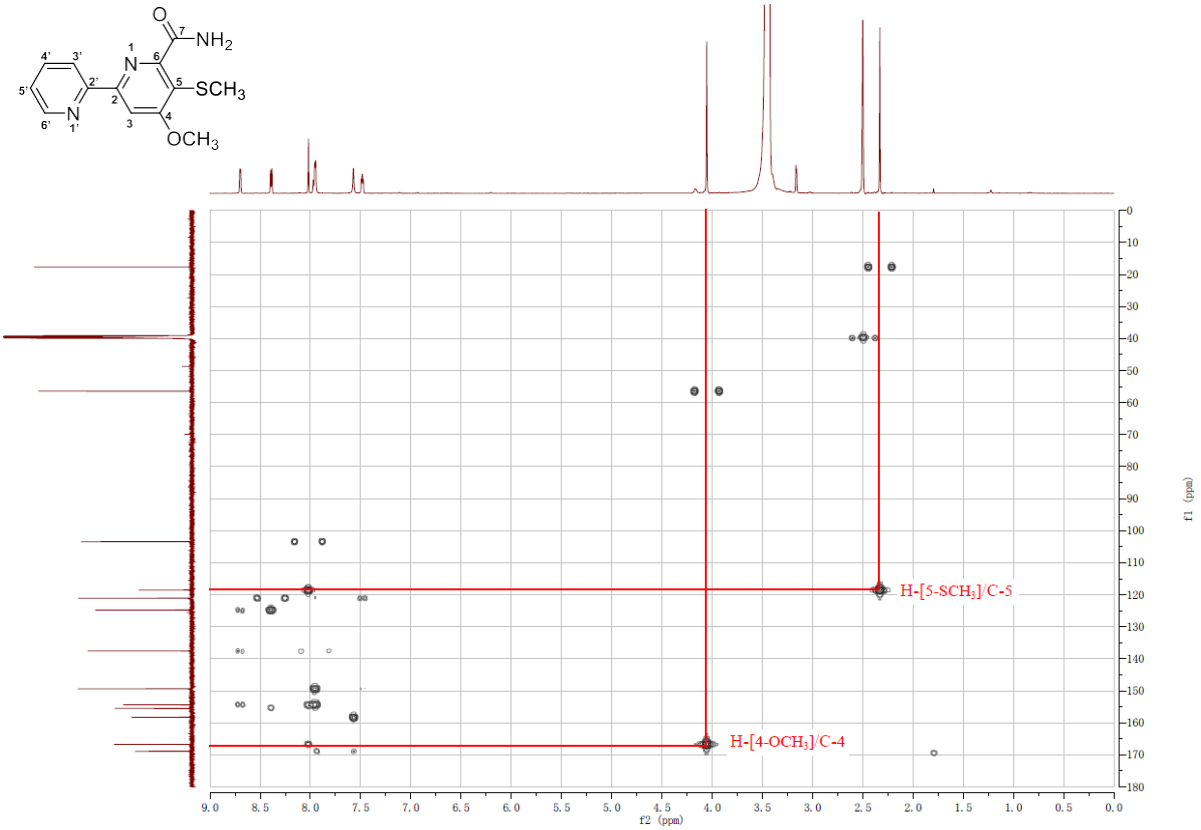


Figure S11: HMBC spectrum of compound **1** (in DMSO-d_6)

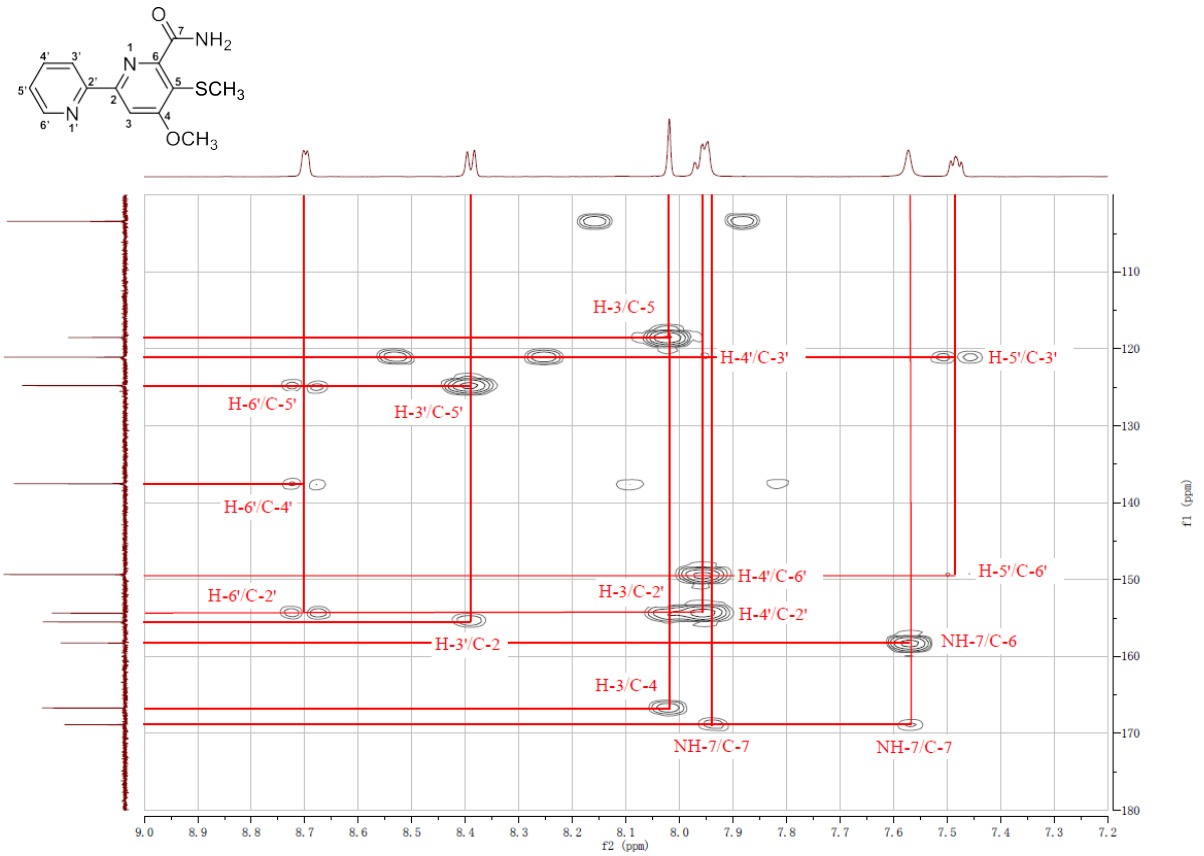


Figure S12: HMBC spectrum of compound **1** (^{1}H NMR from 7.20 to 9.00 ppm, ^{13}C NMR from 100 to 180 ppm)

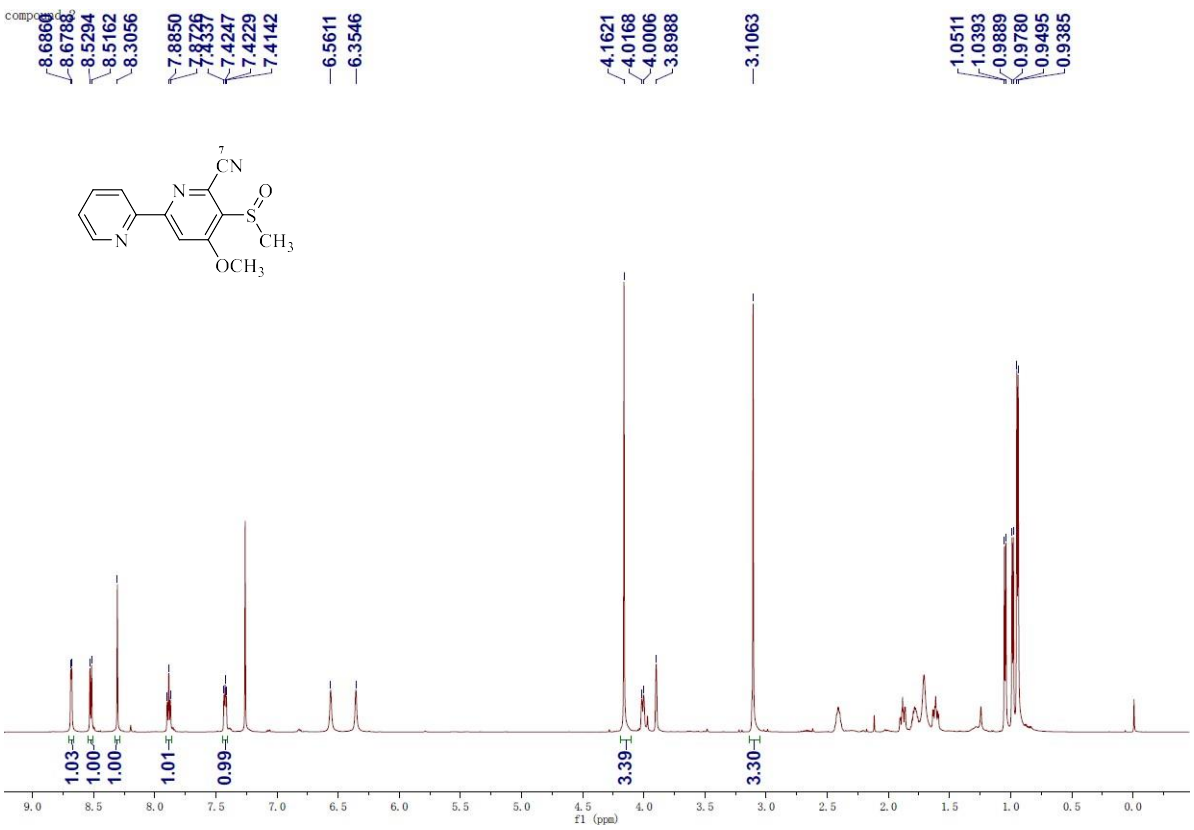


Figure S13: ^{1}H NMR spectrum of compound **2** containing impurities (in $CDCl_3$, 600 MHz)

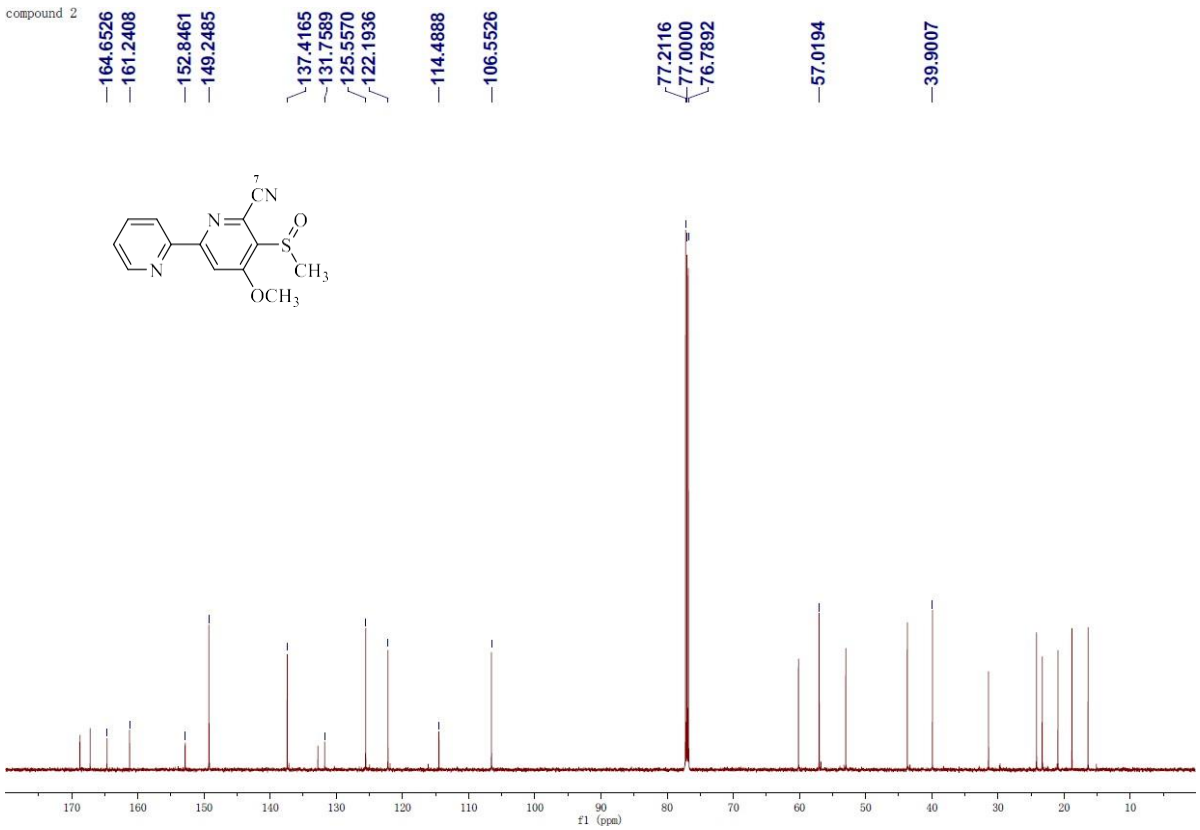


Figure S14: ^{13}C NMR spectrum of compound **2** containing impurities (in $CDCl_3$, 600 MHz)

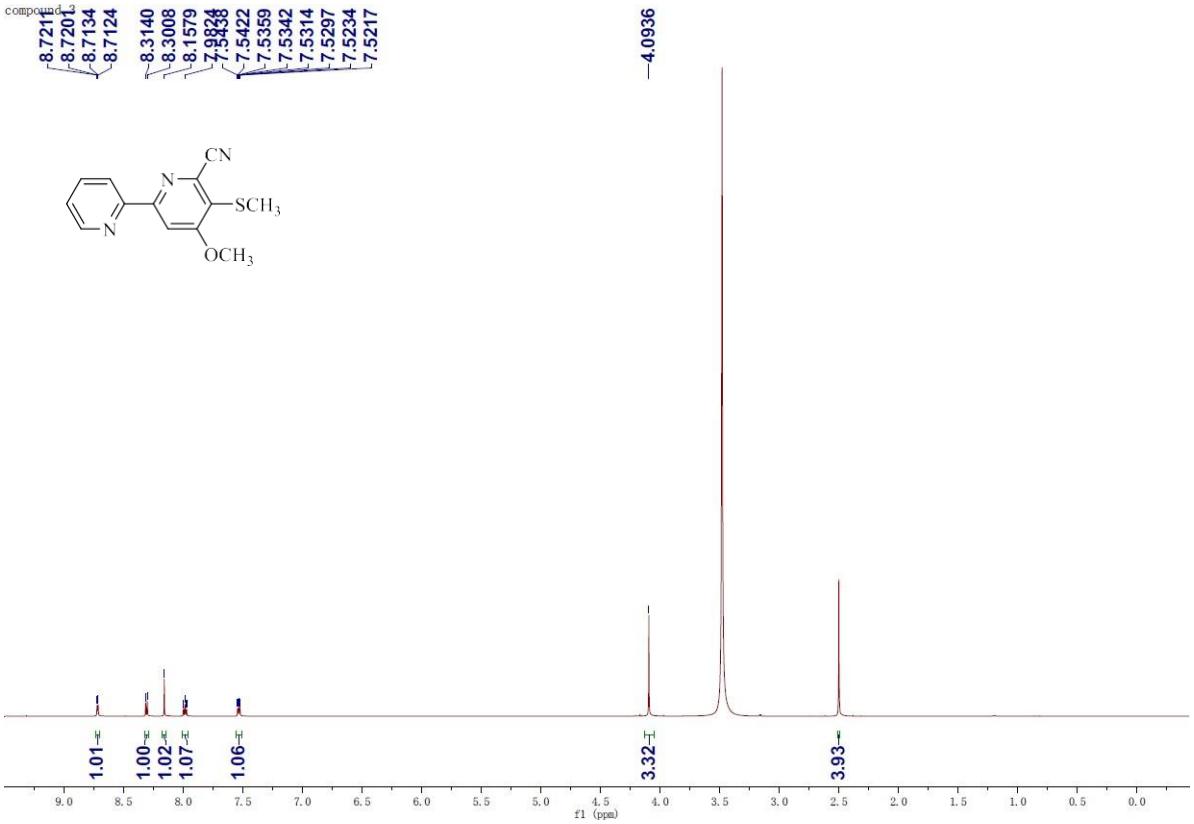


Figure S15: ^{1}H NMR spectrum of compound **3** (in DMSO-d_6, 600 MHz)

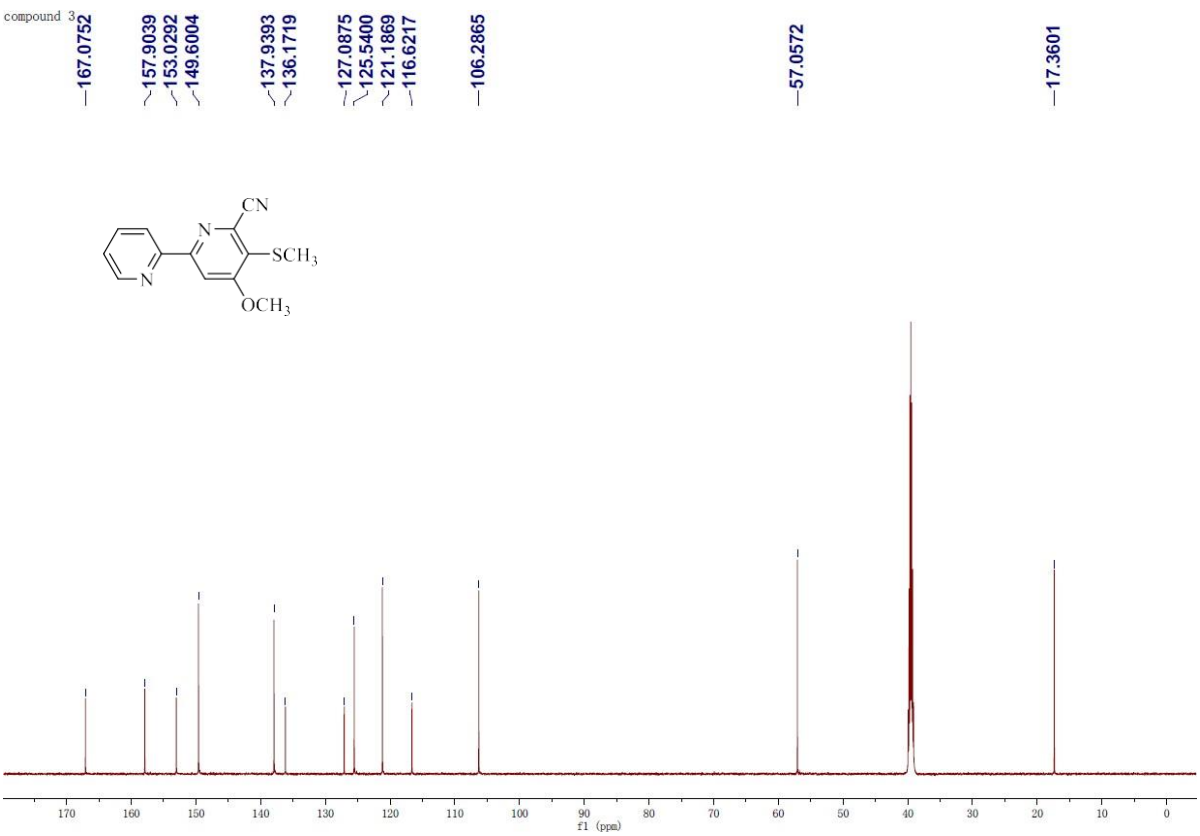


Figure S16: ^{13}C NMR spectrum of compound **3** (in DMSO-d_6, 600 MHz)

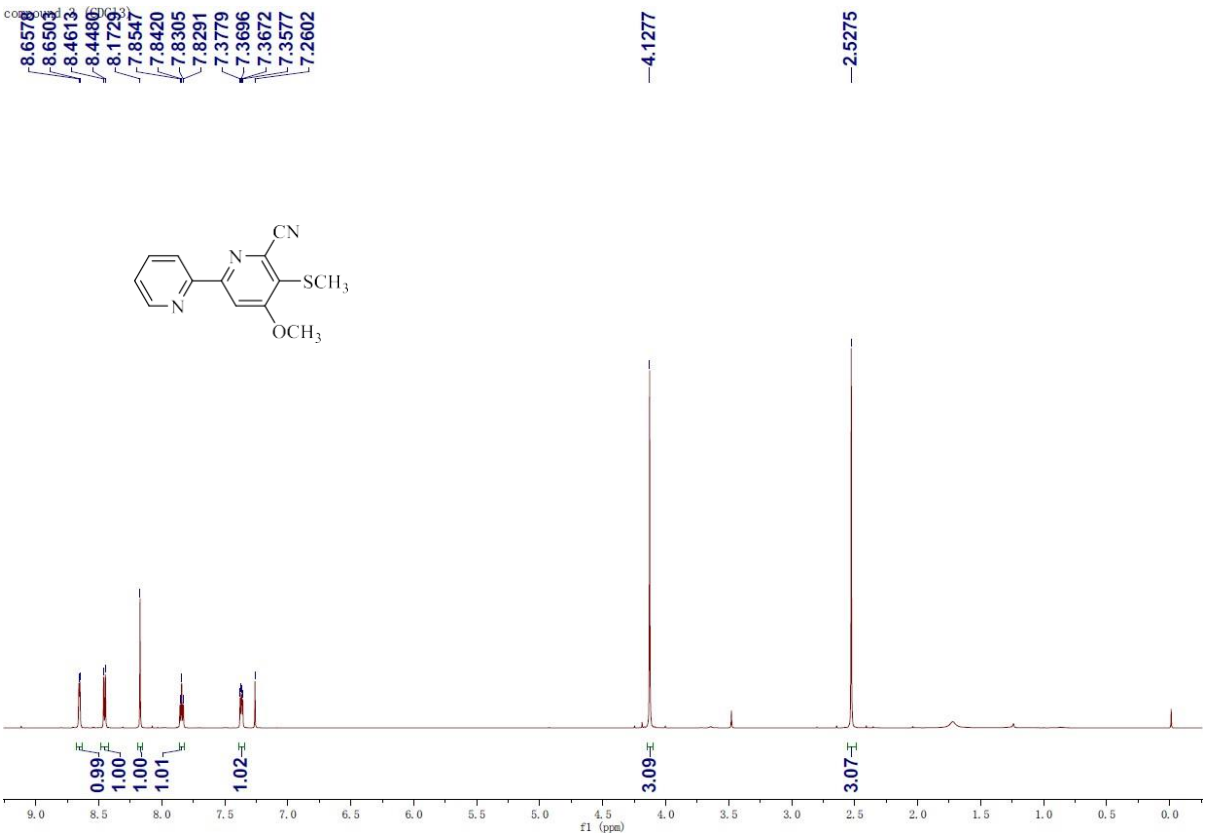


Figure S17: ^{1}H NMR spectrum of compound **3** (in $CDCl_3$, 600 MHz)

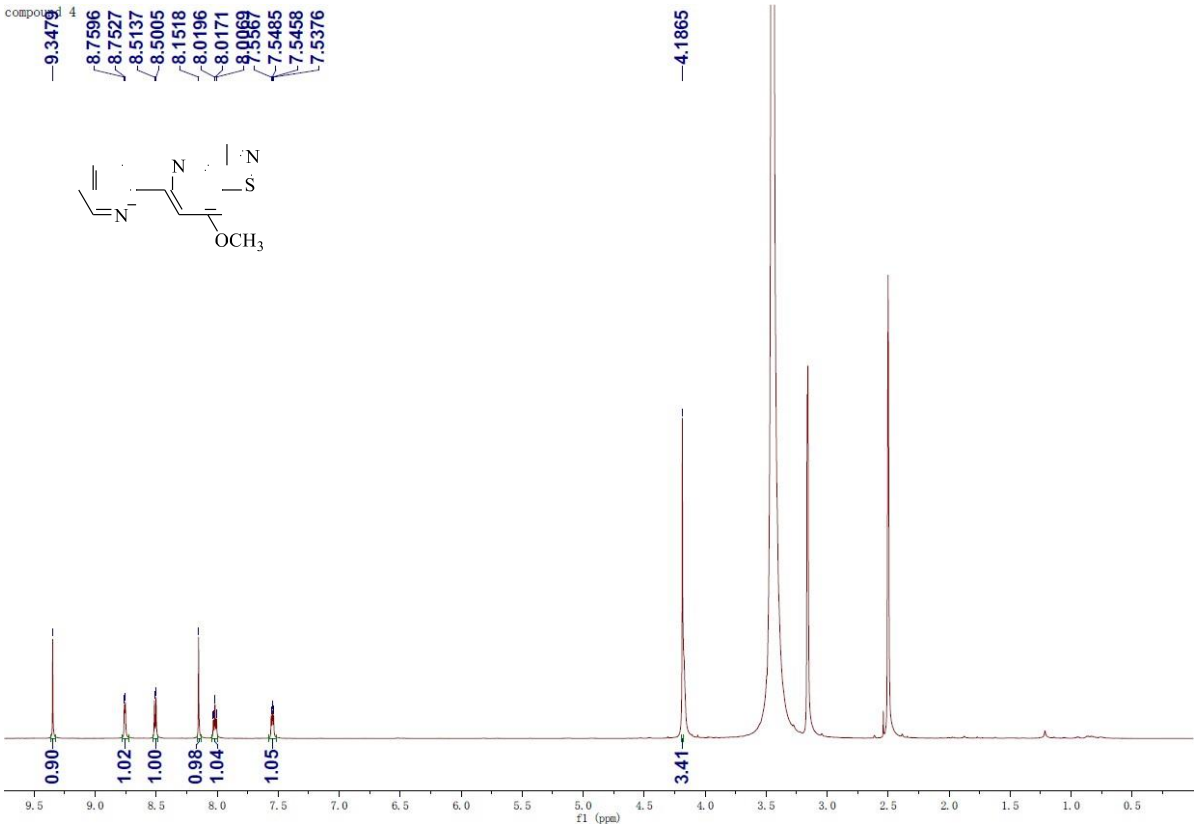


Figure S18: ^{1}H NMR spectrum of compound **4** (in DMSO-d_6, 600 MHz)

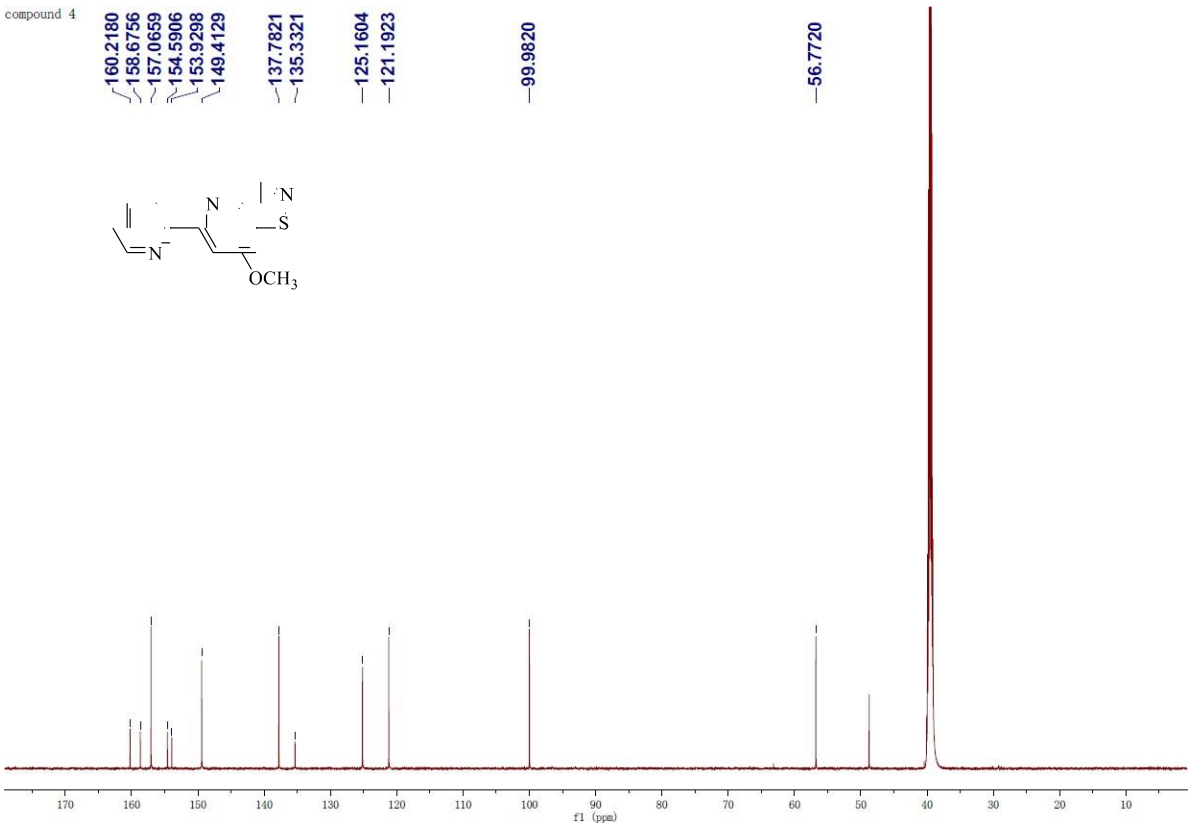


Figure S19: ^{13}C NMR spectrum of compound **4** (in DMSO-d_6, 600 MHz)

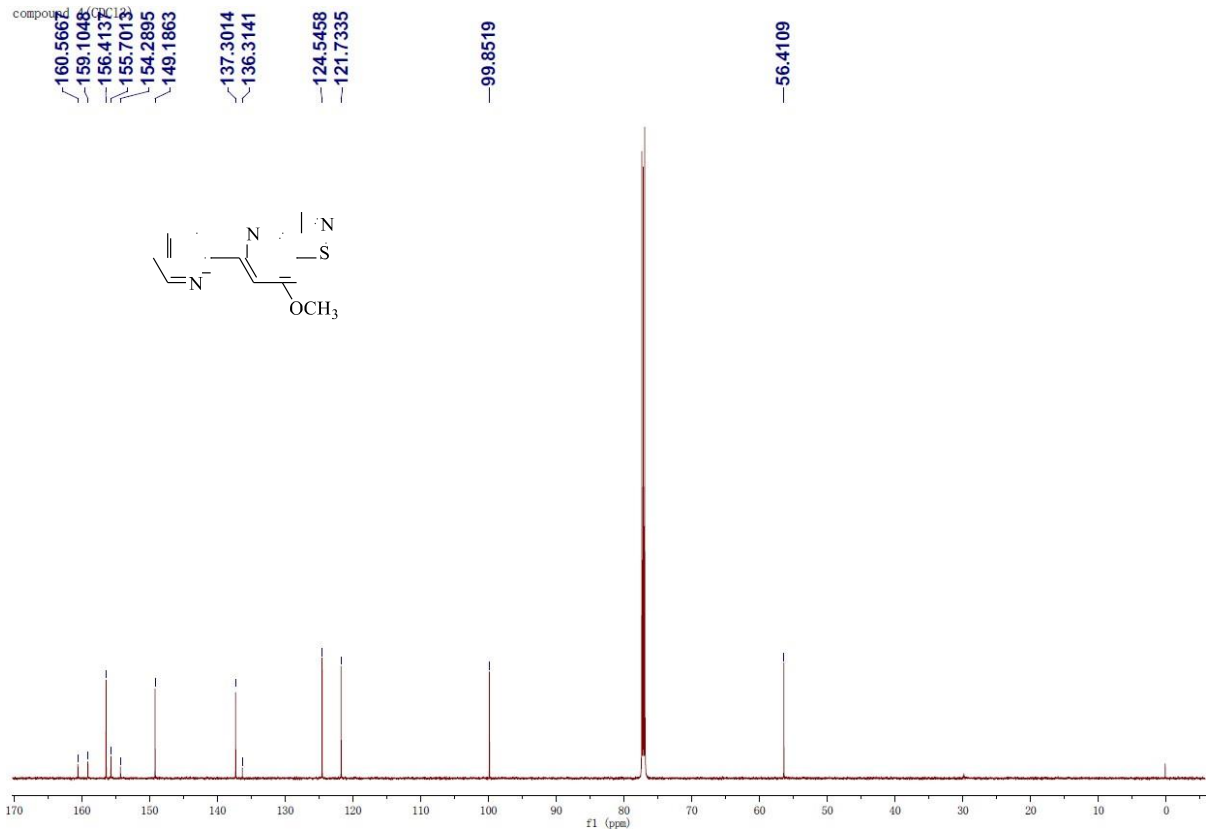
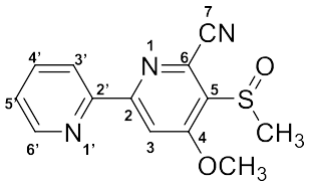


Figure S20: ^{13}C NMR spectrum of compound **4** (in $CDCl_3$, 600 MHz)

Table S1: Comparisons of the NMR data for Pyrisulfoxin B **(2)** between this paper and the literature.

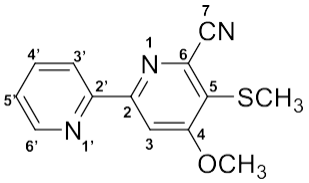
Position	δ_H (ppm, *J* in Hz, in $CDCl_3$)		δc (ppm, in $CDCl_3$)	
	this paper	literature	this paper	literature
2			161.2 (C)	161.2 (C)
3	8.31 (1H, s)	8.29 (1H,s)	106.6 (CH)	106.6 (CH)
4			164.6 (C)	164.7 (C)
4-OCH_3	4.17 (3H, s)	4.15 (3H, s)	57.0 (CH_3)	57.0 (CH_3)
5			131.8 (C)	131.9 (C)
(5-$SOCH_3$)	3.11 (3H, s)	3.09 (3H, s)	39.9 (CH_3)	39.9 (CH_3)
6			137.4 (C)	137.4 (C)
7			114.5 (C)	114.5 (C)
2'			152.8 (C)	152.9 (C)
3'	8.52 (1H, d, *J* = 7.8 Hz)	8.51 (1H, ddd, *J* = 8.0, 1.0, 1.0 Hz)	122.2 (CH)	122.2 (CH)
4'	7.88 (1H, t, *J* = 7.2 Hz)	7.87 (1H, ddd, *J* = 8.0, 7.5, 1.8 Hz)	137.4 (CH)	137.4 (CH)
5'	7.42 (1H, dd, *J* = 6.6, 5.4 Hz)	7.40 (1H, ddd, *J* = 7.5, 4.9, 1.1 Hz)	125.6 (CH)	125.5 (CH)
6'	8.68 (1H, d, *J* = 4.2 Hz)	8.67 (1H, ddd, *J* = 4.8, 1.8, 1.0 Hz)	149.2 (CH)	149.2 (CH)



Pyrisulfoxin B **(2)**

Table S2: Comparisons of the NMR data for SF2738D **(3)** between this paper and the literature

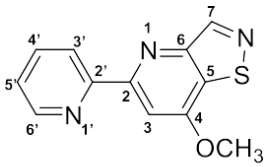
Position	δ_H (ppm, *J* in Hz)			δc (ppm, $CDCl_3$)	
	this paper (in DMSO-d_6)	this paper (in $CDCl_3$)	literature (in CDCl3)	this paper (in DMSO-d6)	literature (in CDCl3)
2				157.9 (C)	158.5 (C)
3	8.16 (1H, s)	8.18 (1H, s)	8.20 (1H,s)	106.3 (CH)	105.7 (CH)
4				167.1 (C)	167.0 (C)
4-OCH_3	4.09 (3H, s)	4.14 (3H, s)	4.15 (3H, s)	57.0 (CH_3)	56.6
5				127.1 (C)	127.3 (C)
(5-SCH_3)	2.50 (3H, s)	2.54 (3H, s)	2.55 (3H, s)	17.4 (CH_3)	17.9
6				137.9 (C)	137.6 (C)
7				116.6 (C)	116.5 (C)
2'				153.0 (C)	153.8 (C)
3'	8.31 (1H, d, *J* = 7.8 Hz)	8.46 (1H, d, *J* = 7.8 Hz)	8.48 (1H, ddd, *J* = 8.0, 1.0, 1.0 Hz)	121.2 (CH)	121.7 (CH)
4'	7.98 (1H, td, *J* = 7.8 , 1.8 Hz)	7.86 (1H, td, *J* = 7.8, 0.6 Hz)	7.86 (1H, ddd, *J* = 8.0, 7.4, 1.8 Hz)	136.2 (CH)	137.2 (CH)
5'	7.53 (1H, ddd, *J* = 7.8, 4.8, 1.2 Hz)	7.38 (1H, dd, *J* = 6.6, 4.8 Hz)	7.38 (1H, ddd, *J* = 7.5, 4.9, 1.0 Hz)	125.5 (CH)	124.8 (CH)
6'	8.72 (1H, ddd, *J* = 4.8, 1.8, 1.2 Hz)	8.67 (1H, d, *J* = 4.8 Hz)	8.67 (1H, ddd, *J* = 4.8, 1.8, 1.0 Hz)	149.6 (CH)	149.1 (CH)



SF2738D **(3)**

Table S3: Comparisons of the NMR data for SF2738F **(4)** between this paper and the literature.

Position	δ_H (ppm, *J* in Hz)		δc (ppm, $CDCl_3$)		
	this paper (in DMSO-d_6)	literature (in $CDCl_3$)	this paper (in DMSO-d_6)	this paper (in $CDCl_3$)	literature (in $CDCl_3$)
2			158.7 (C)	159.1 (C)	158.9 (C)
3	8.15 (1H, s)	8.10 (1H, s)	100.0 (CH)	99.8 (CH)	99.7 (CH)
4			160.2 (C)	160.6 (C)	160.4 (C)
4-OCH_3	4.19 (3H, s)	4.20 (3H, s)	56.8 (CH_3)	56.4 (CH3)	56.2 (CH3)
5			135.3 (C)	136.3 (C)	136.1 (C)
6			153.9 (C)	154.3 (C)	154.2 (C)
7	9.35 (1H, s)	9.13 (1H, s)	157.1 (CH)	156.4 (CH)	156.2 (CH)
2'			154.6 (C)	155.7 (C)	155.6 (C)
3'	8.50 (1H, d, *J* = 8.4 Hz)	8.56 (1H, ddd, *J* = 8.0, 1.0, 1.0 Hz)	121.2 (CH)	121.7 (CH)	121.6 (CH)
4'	8.02 (1H, td, *J* = 7.8, 1.8 Hz)	7.88 (1H, ddd, *J* = 8.0, 7.4, 1.8 Hz)	137.8 (CH)	137.3 (CH)	137.1 (CH)
5'	7.56 (1H, ddd, *J* = 7.8, 4.8, 1.2 Hz)	7.38 (1H, ddd, *J* = 7.4, 4.9, 1.0 Hz)	125.2 (CH)	124.5 (CH)	124.3 (CH)
6'	8.75 (1H, d, *J* = 4.2 Hz)	8.56 (1H, ddd, *J* = 4.9, 1.8, 1.0 Hz)	149.4 (CH)	149.2 (CH)	149.0 (CH)



SF2738F **(4)**