marine drugs

MDPI

Supporting information

Halo- and Thiocarbazomycins from Coral- and Coral Reef Sands-Derived *Actinomycetes*

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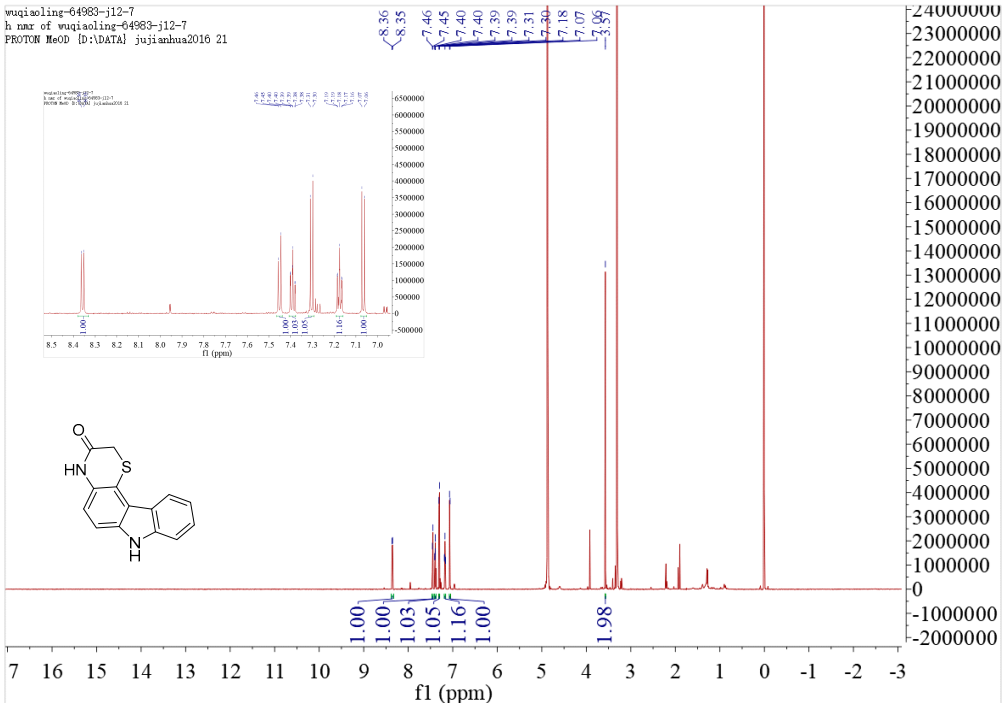
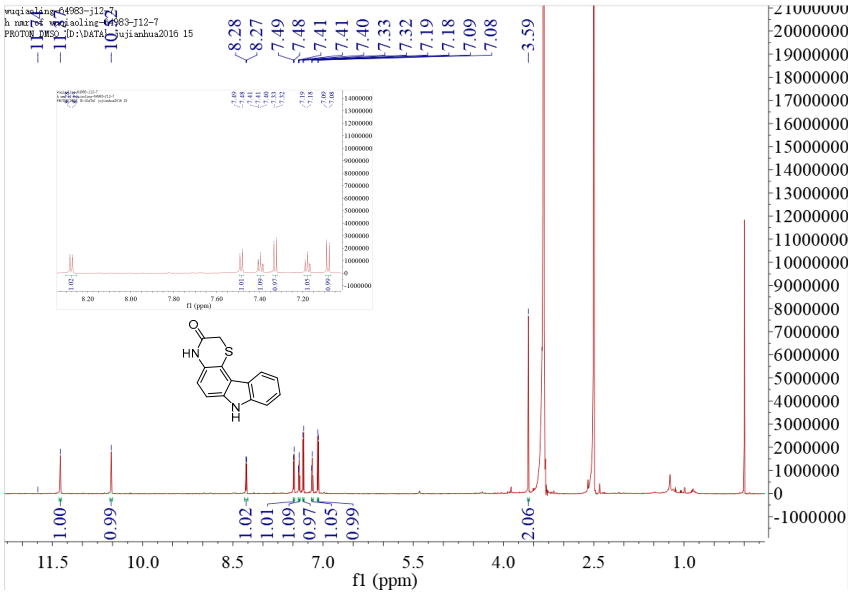


Figure S1. ^{1}H-NMR spectrum of compound **1** in mathanol-d_4.



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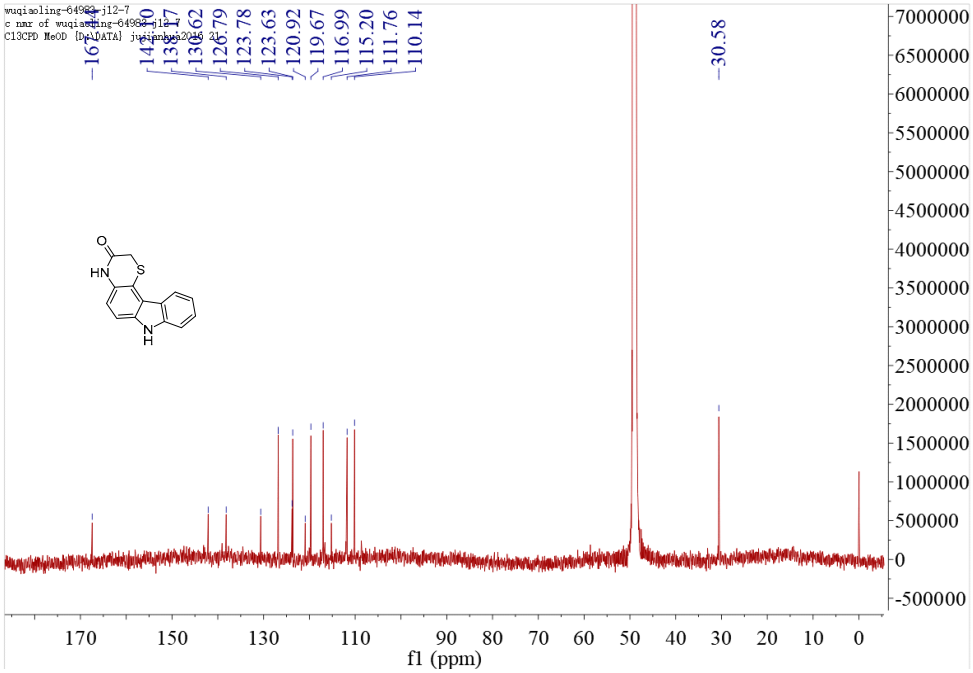

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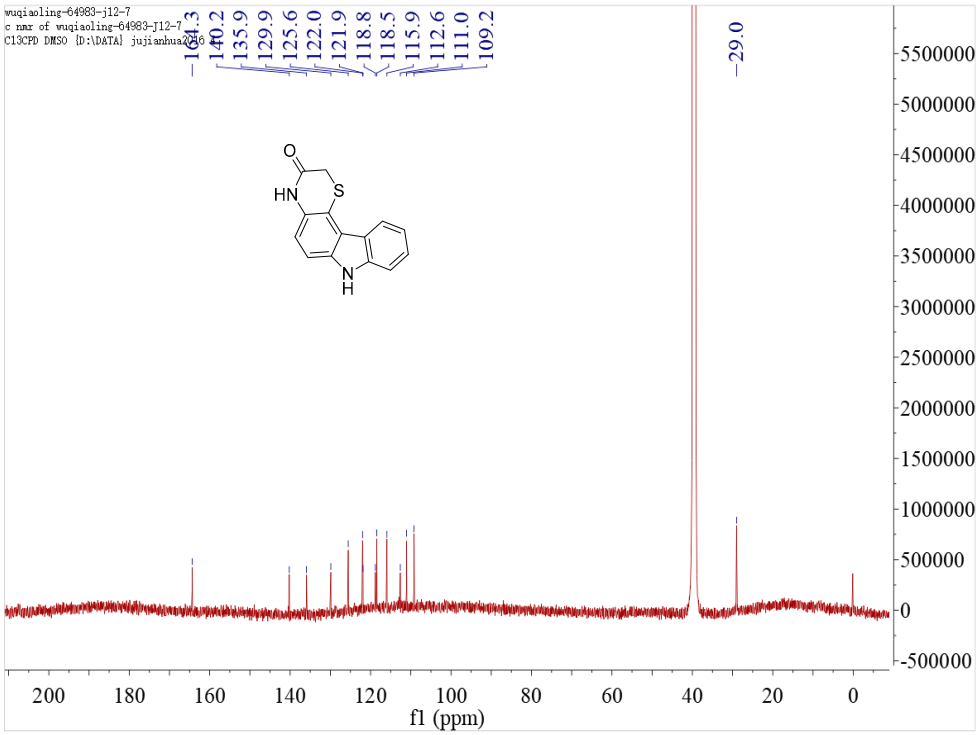

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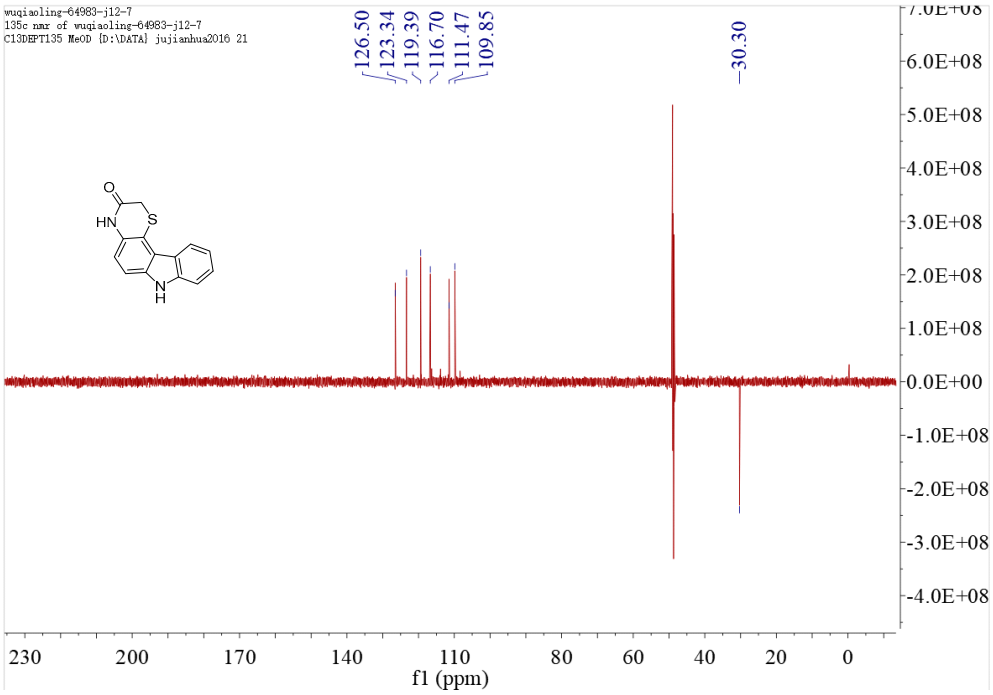

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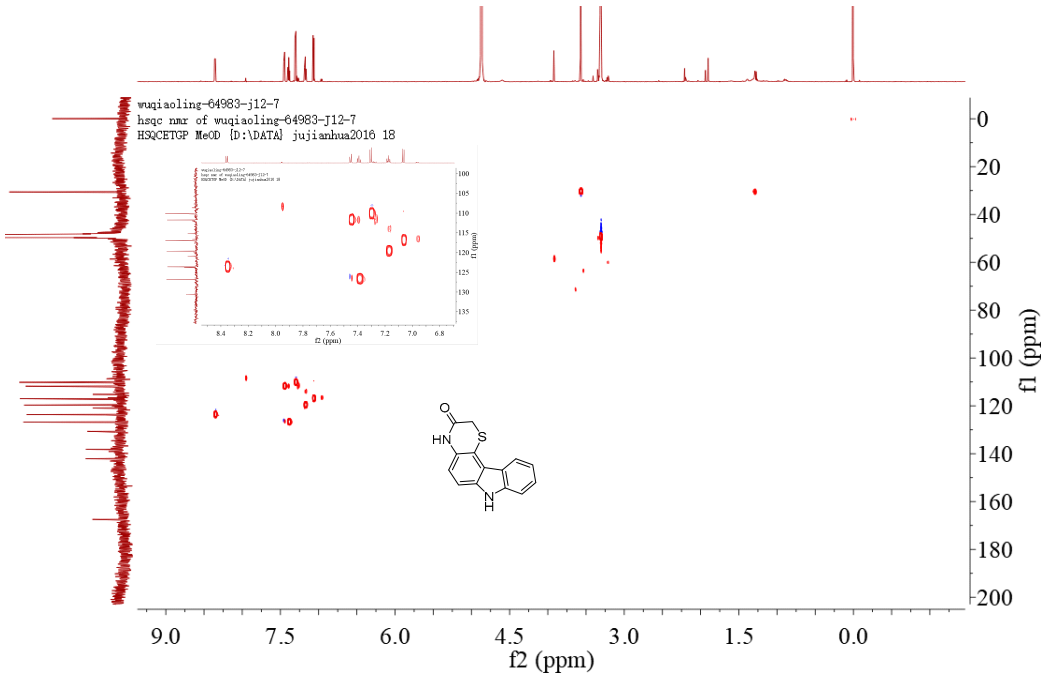

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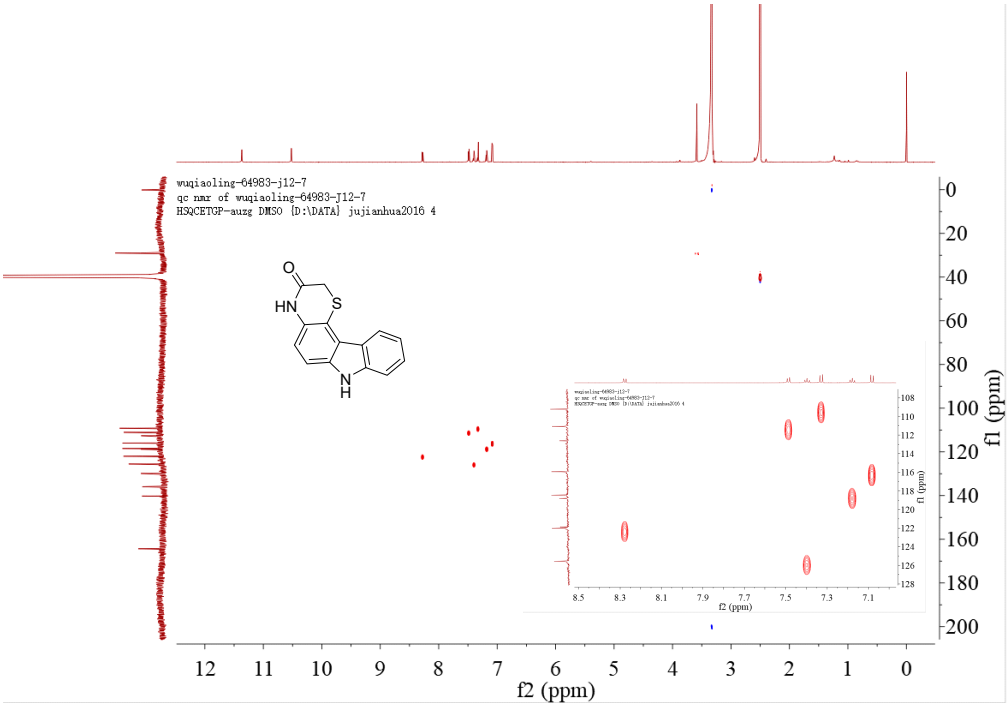

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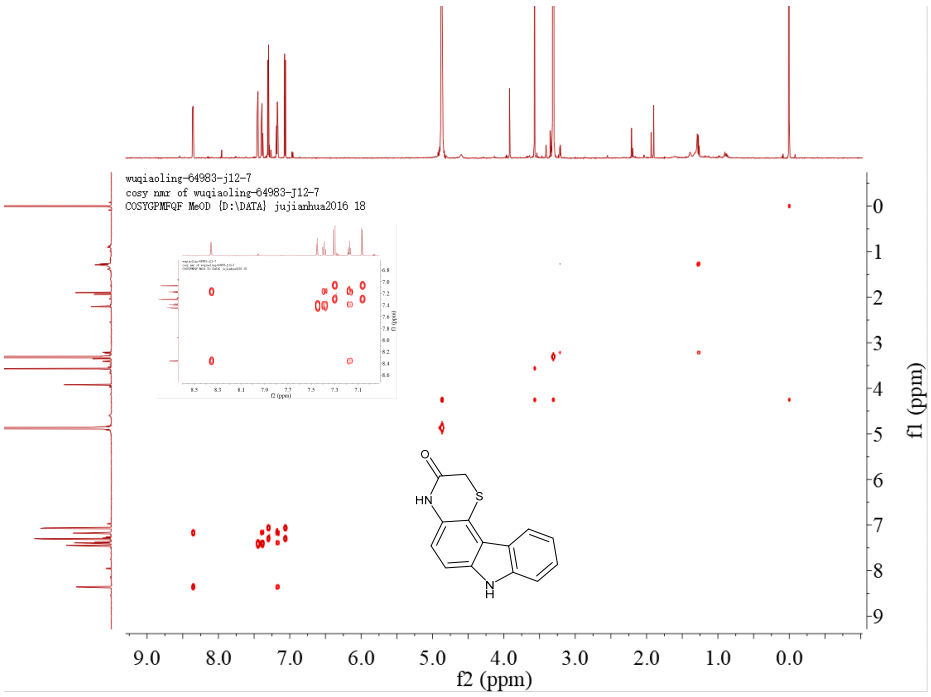

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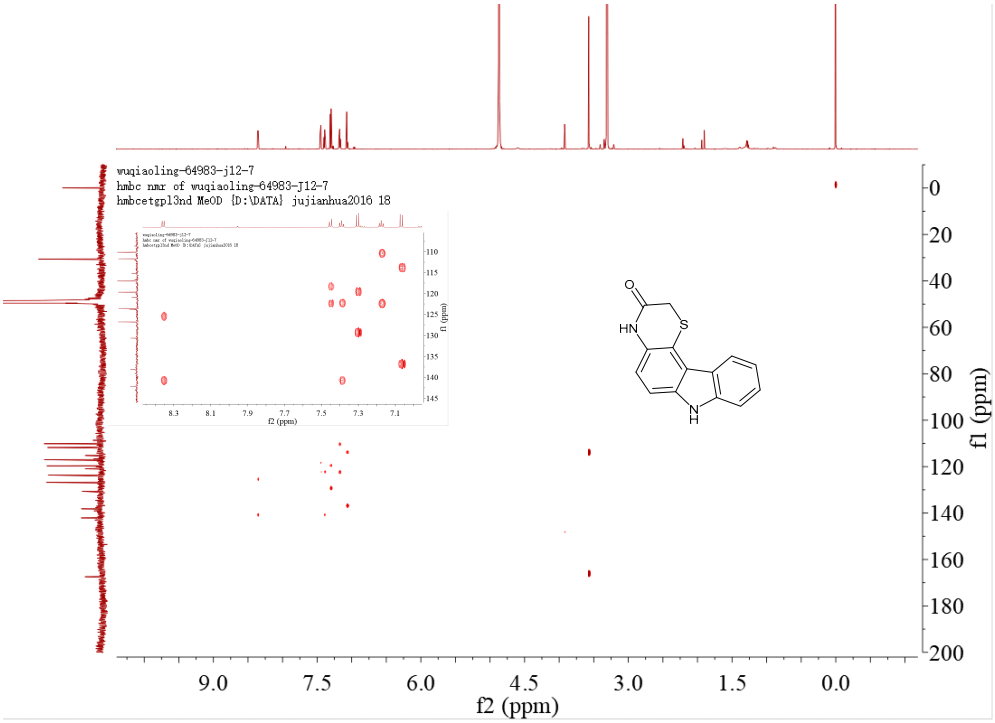

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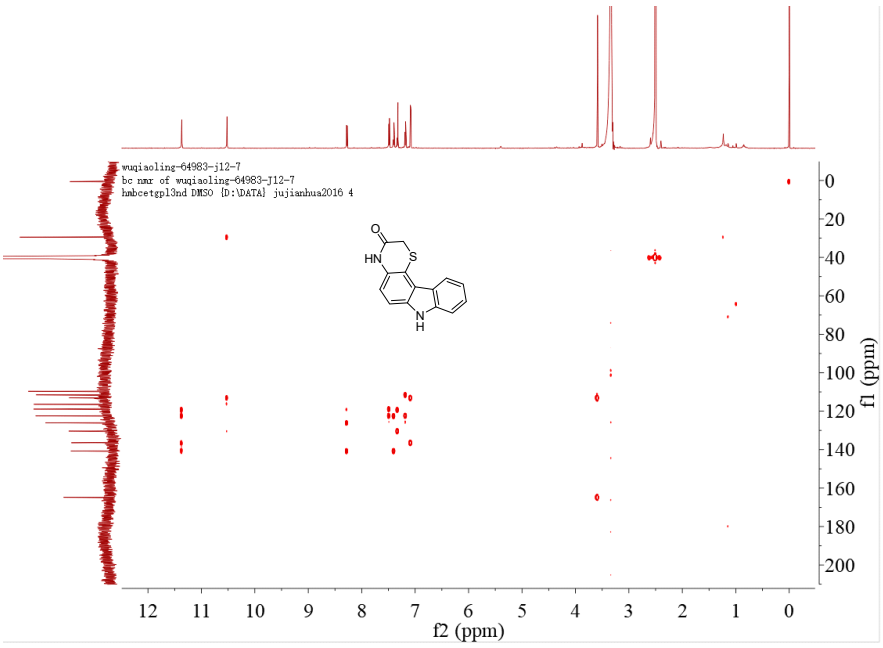

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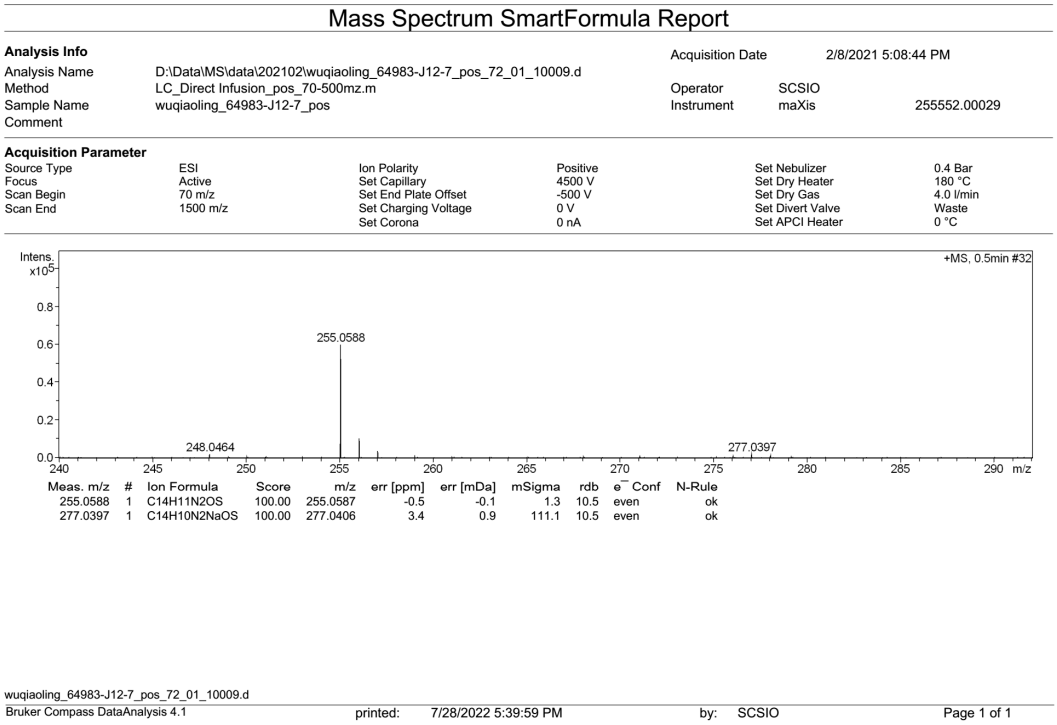

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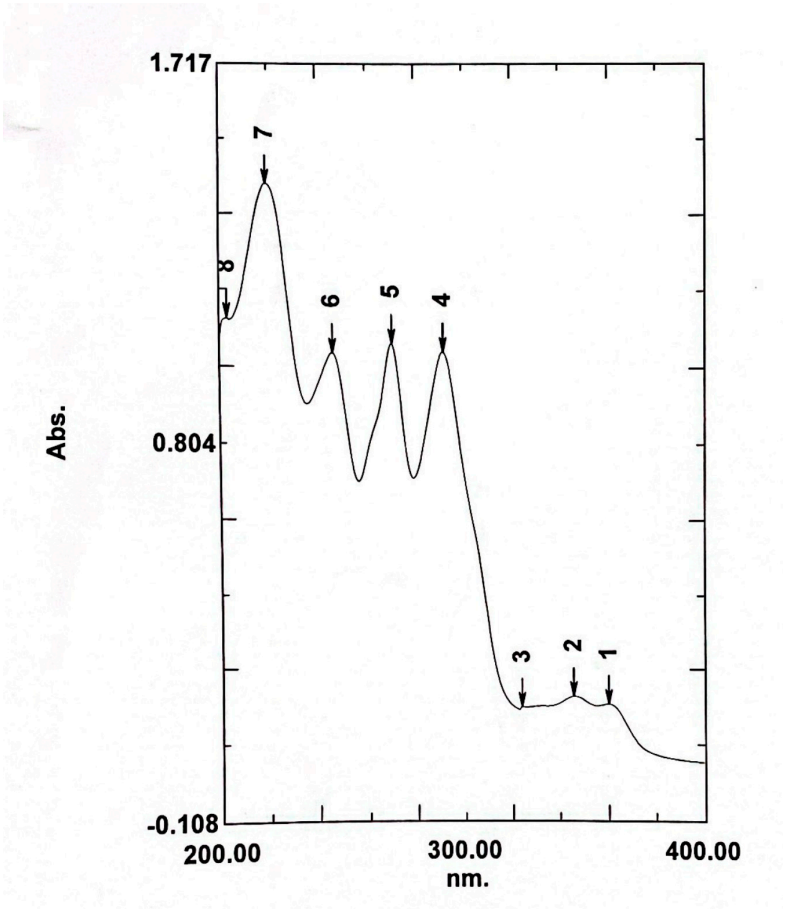

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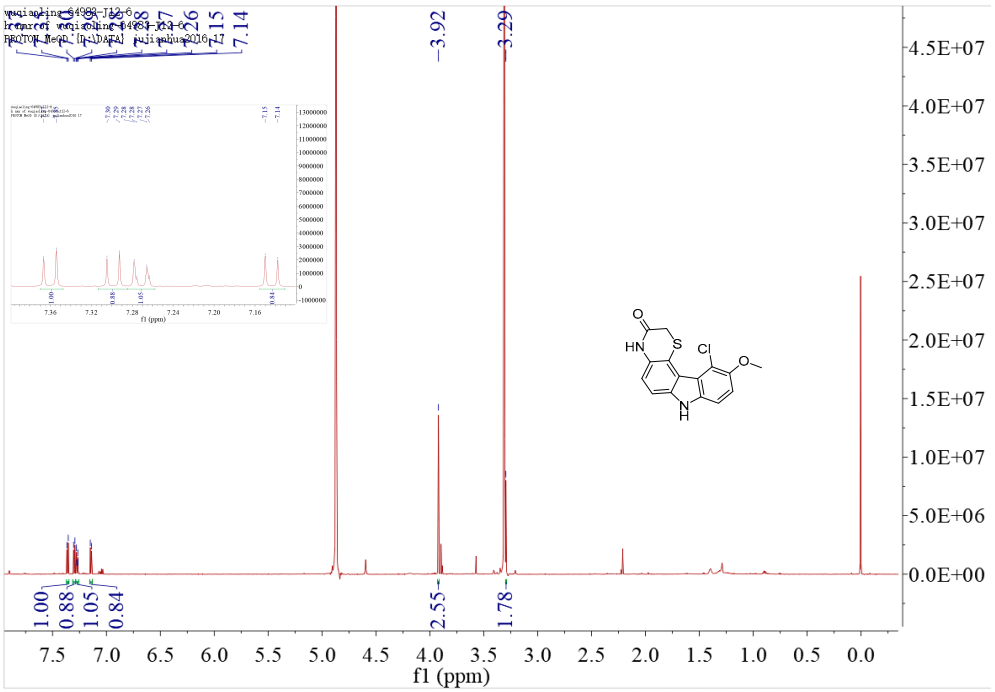

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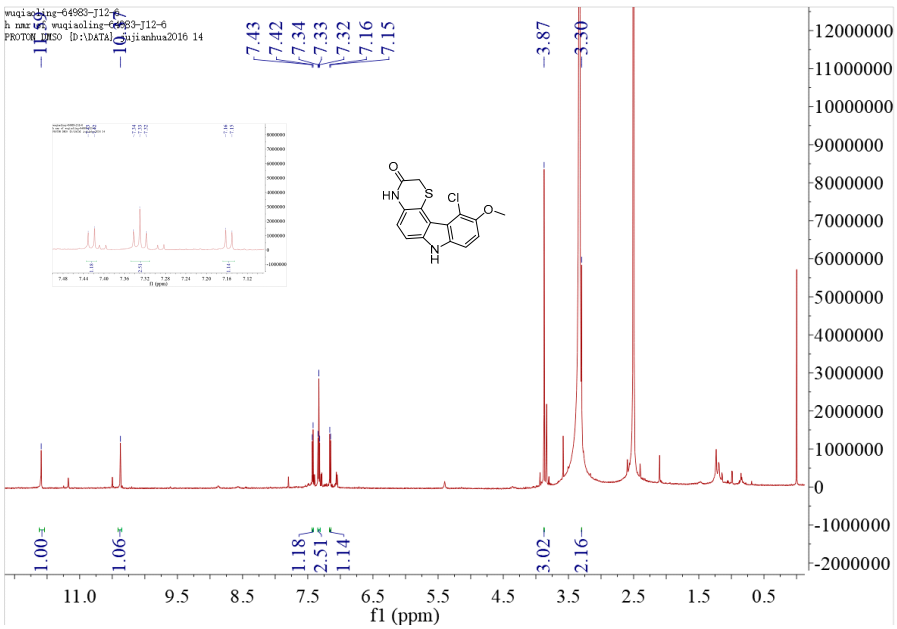

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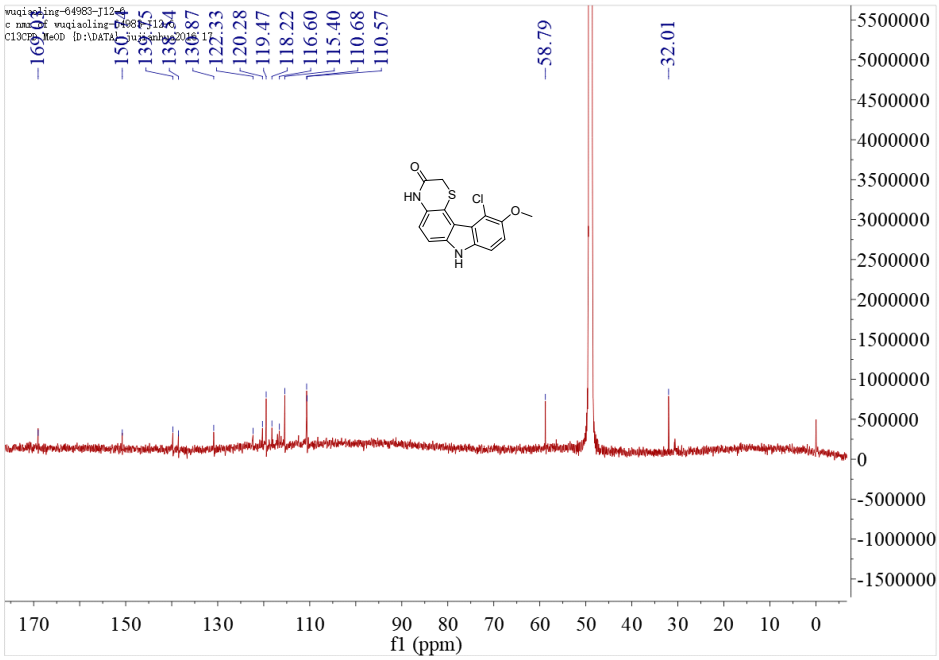

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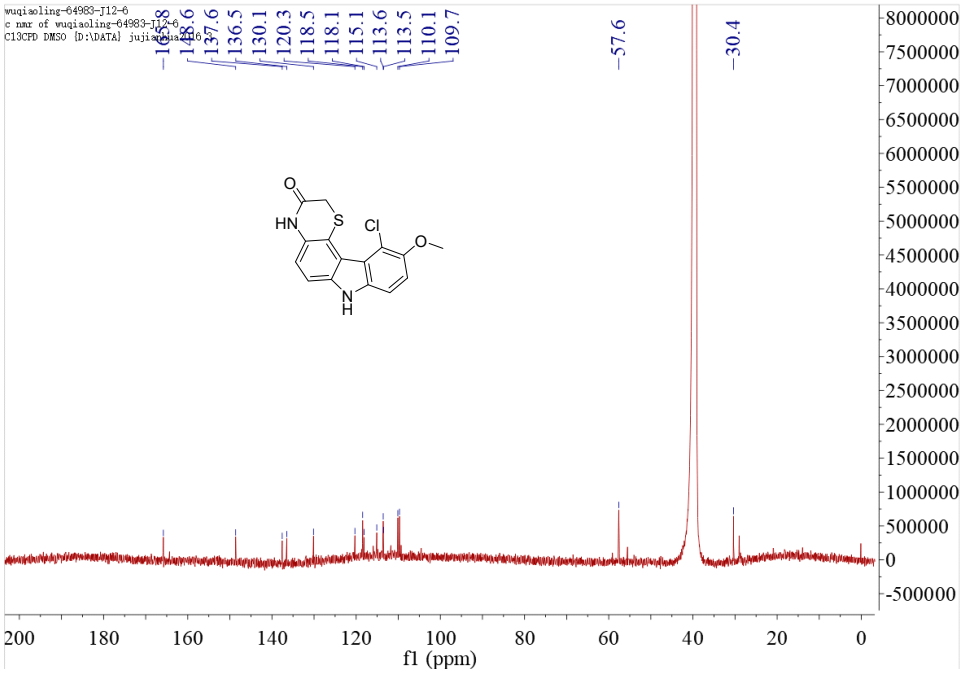

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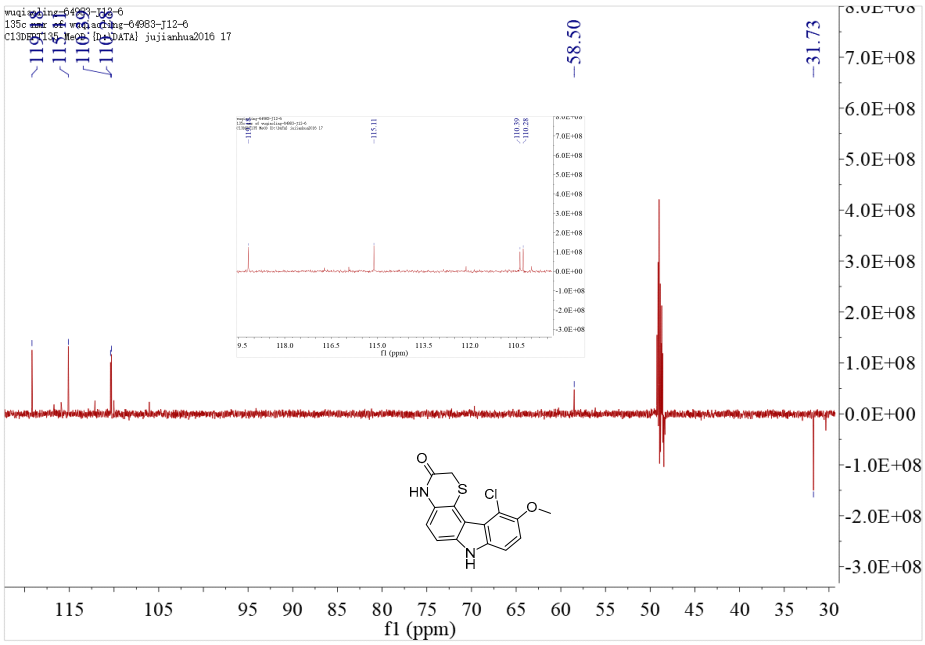

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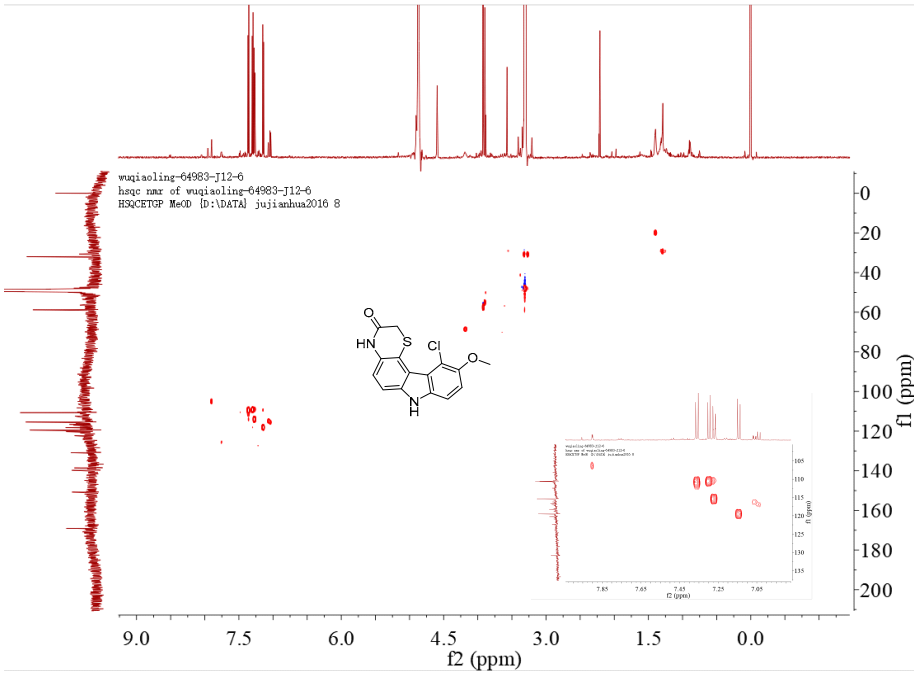

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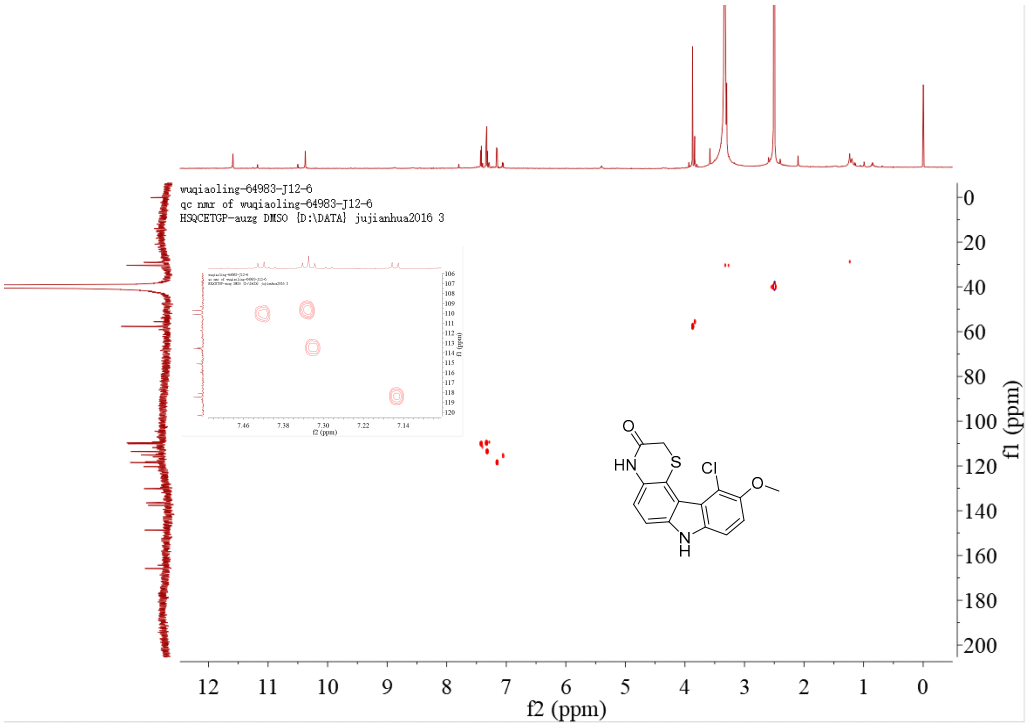

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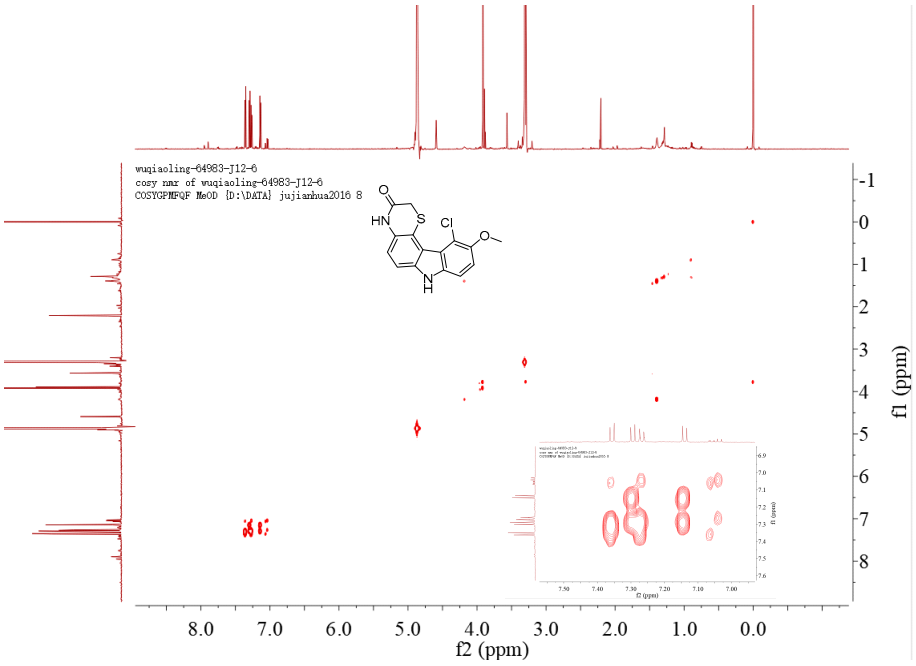

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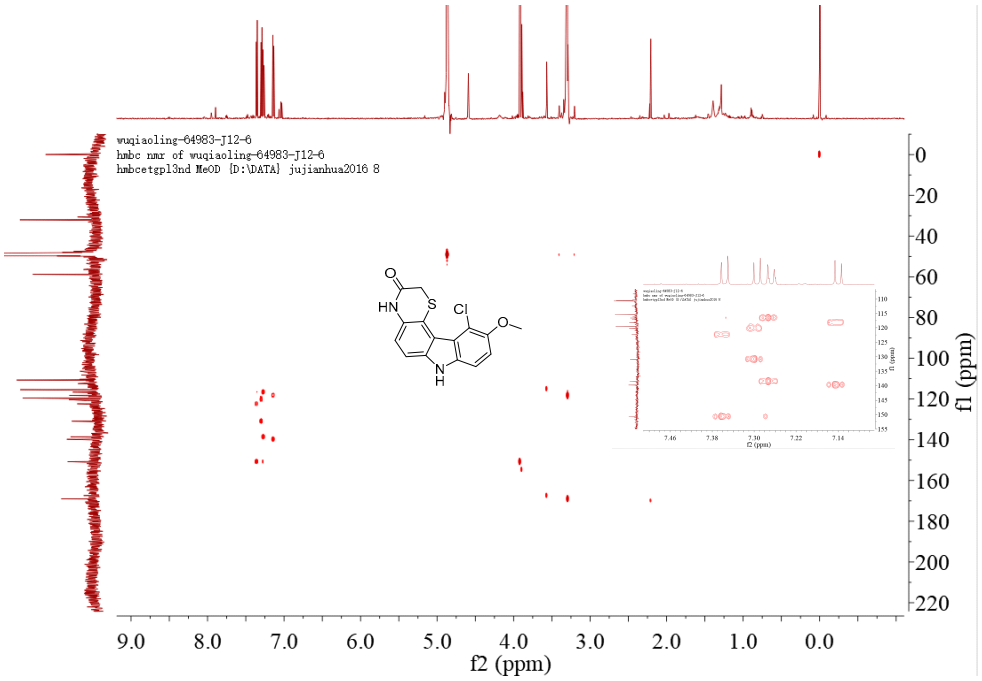

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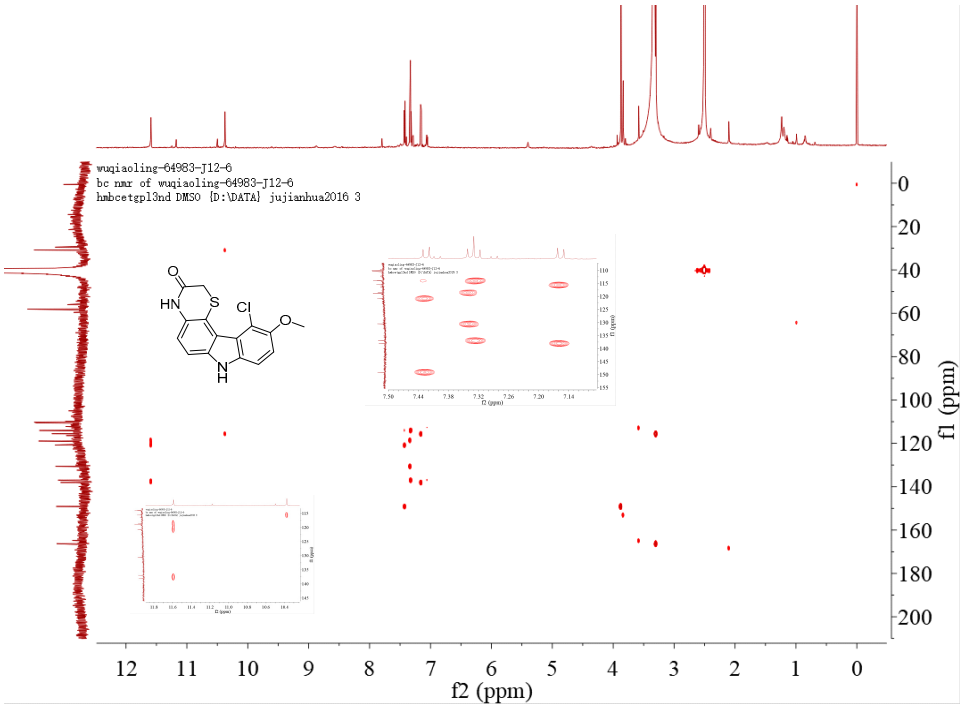

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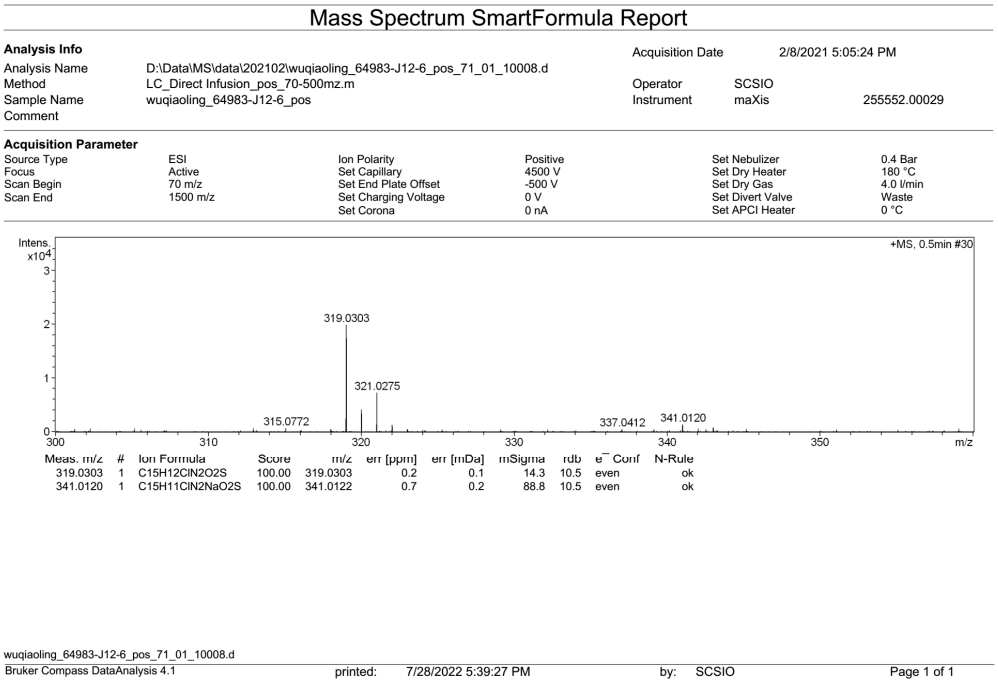

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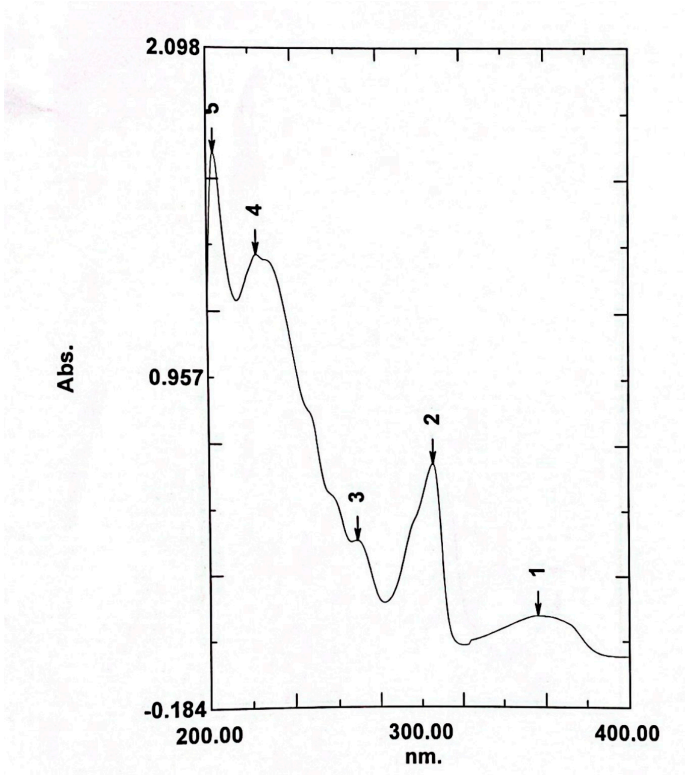

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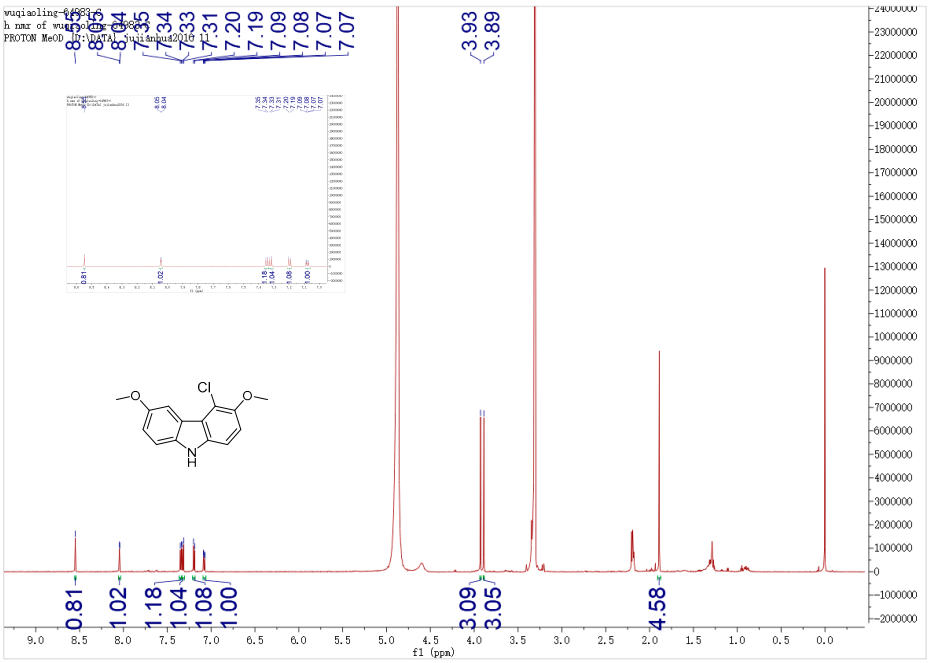

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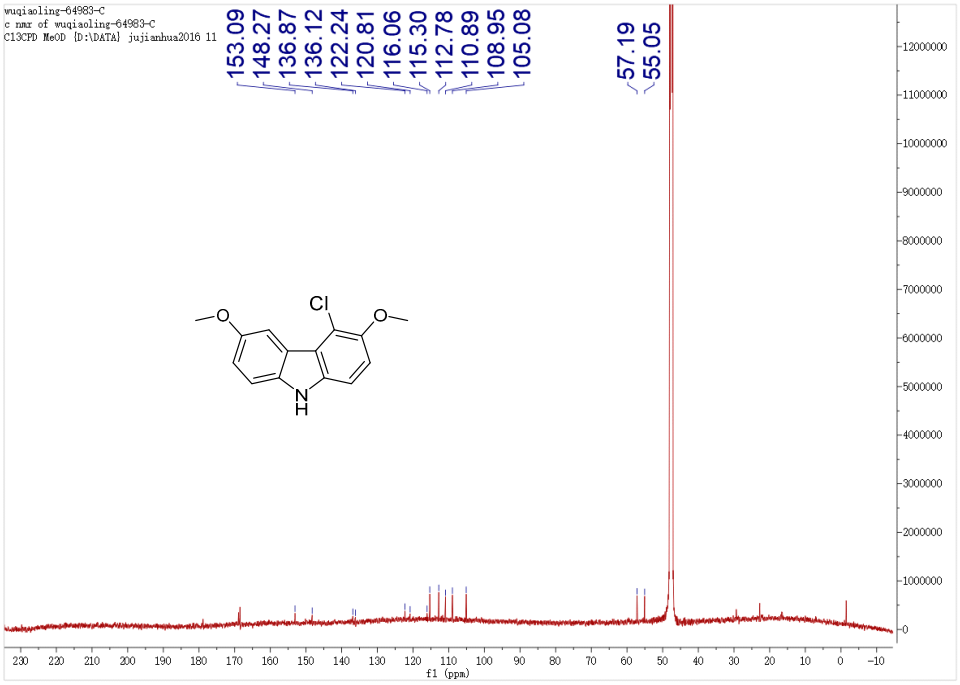

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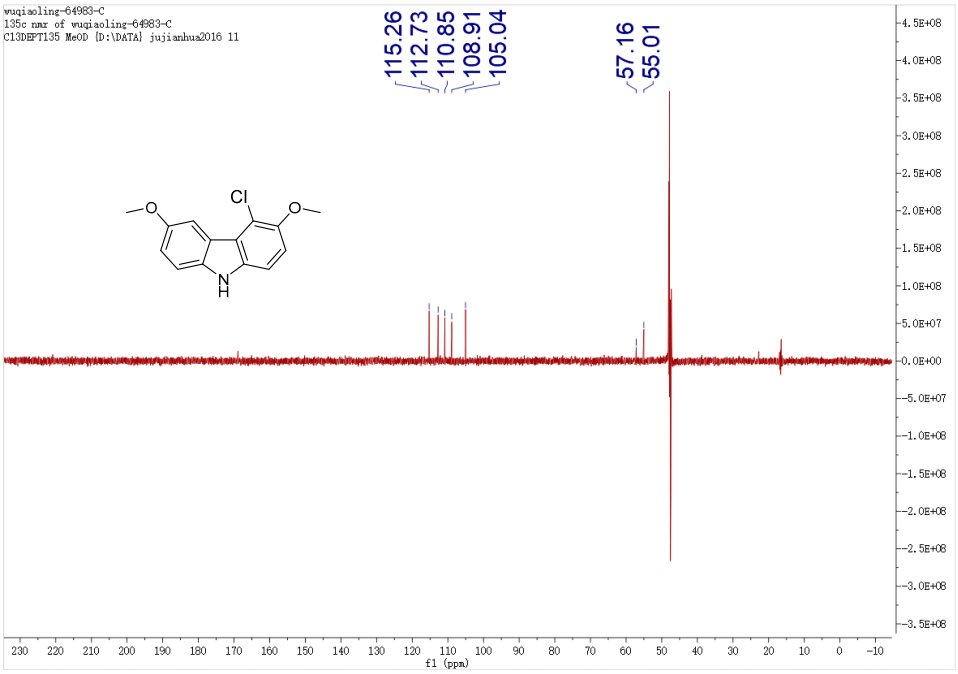

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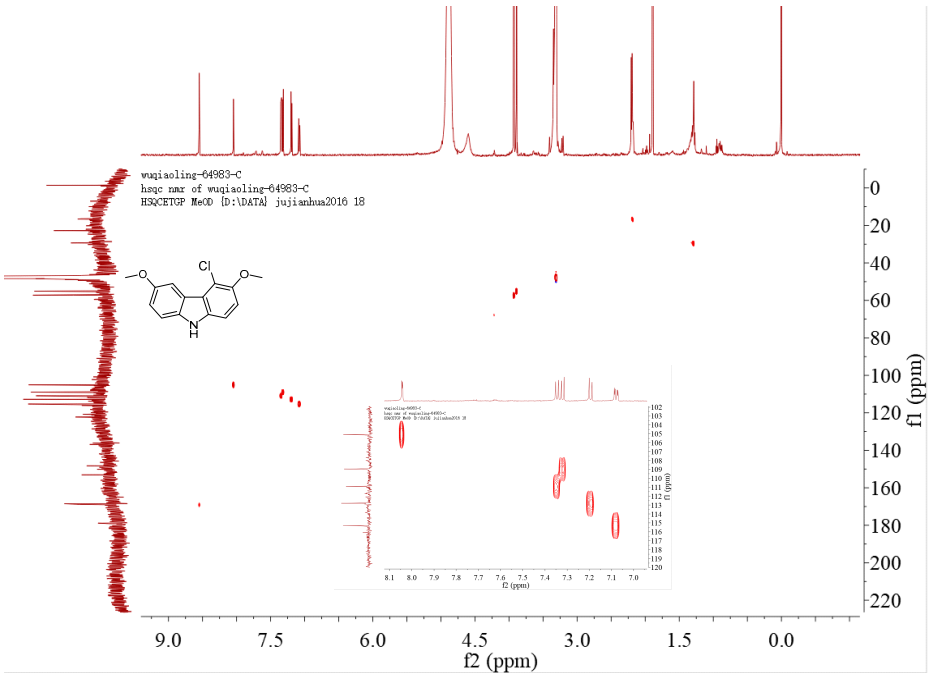

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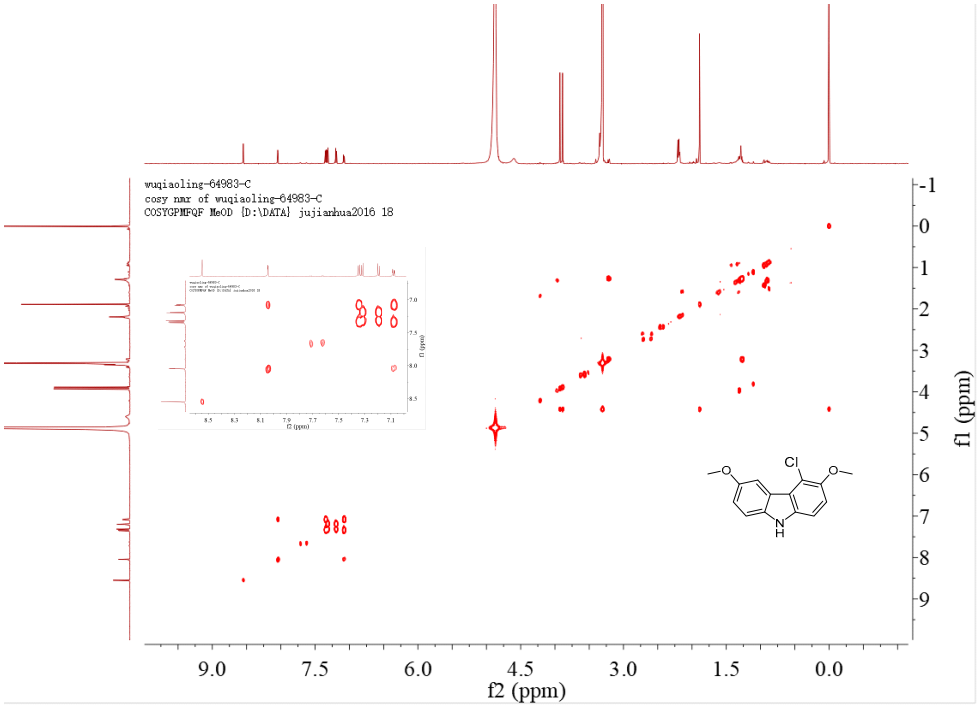
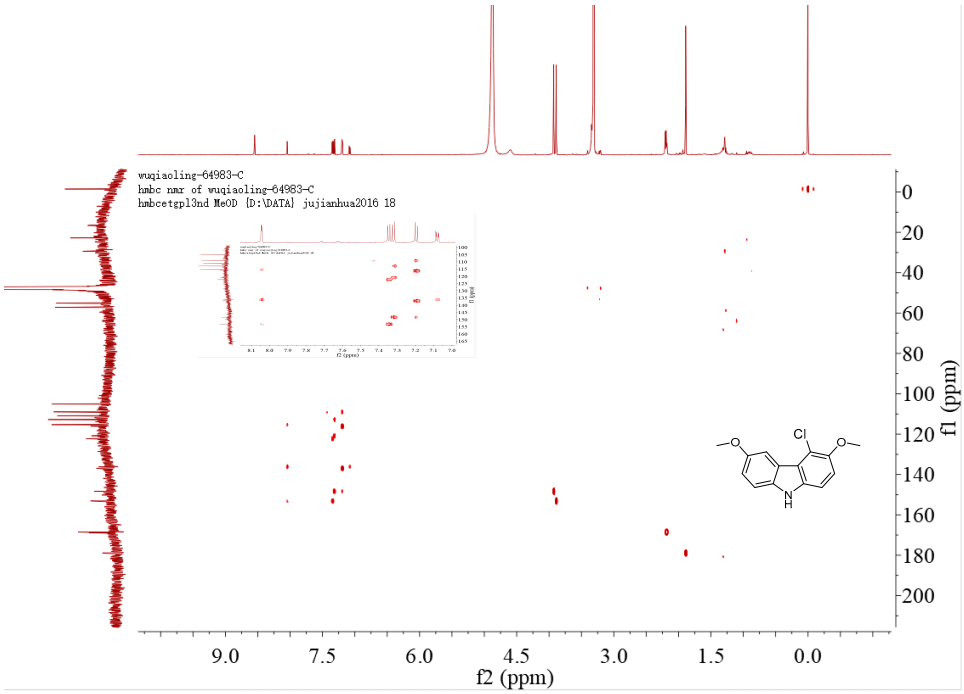


Figure S29.^{1}H-^{1}H COSY spectrum of compound 3 in mathanol-d_4.



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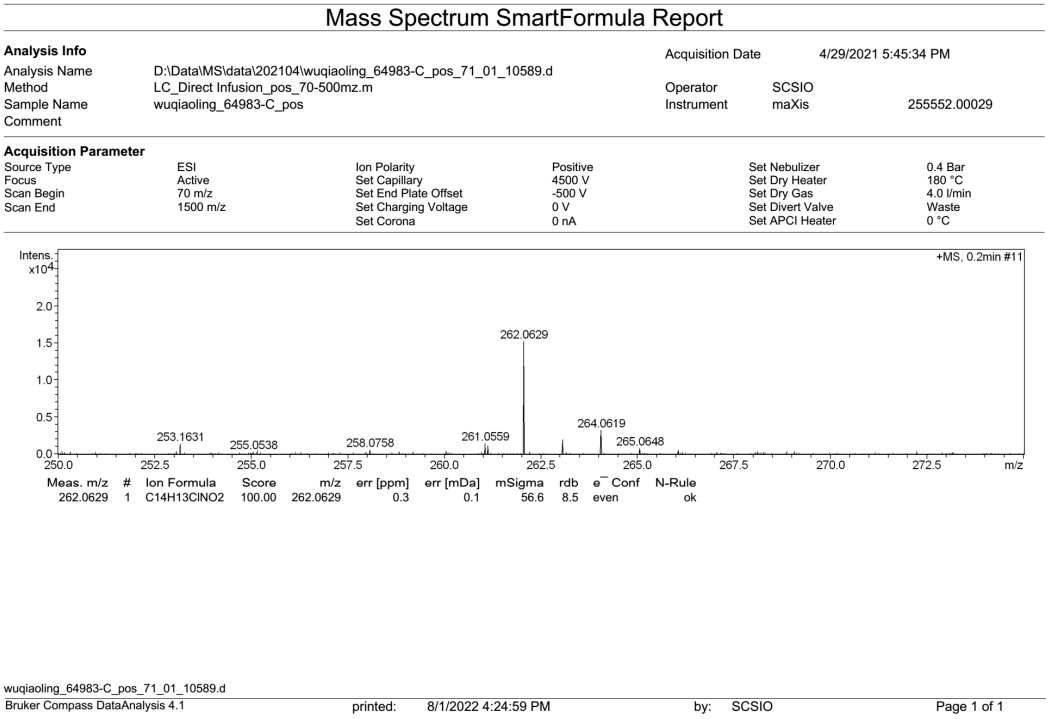

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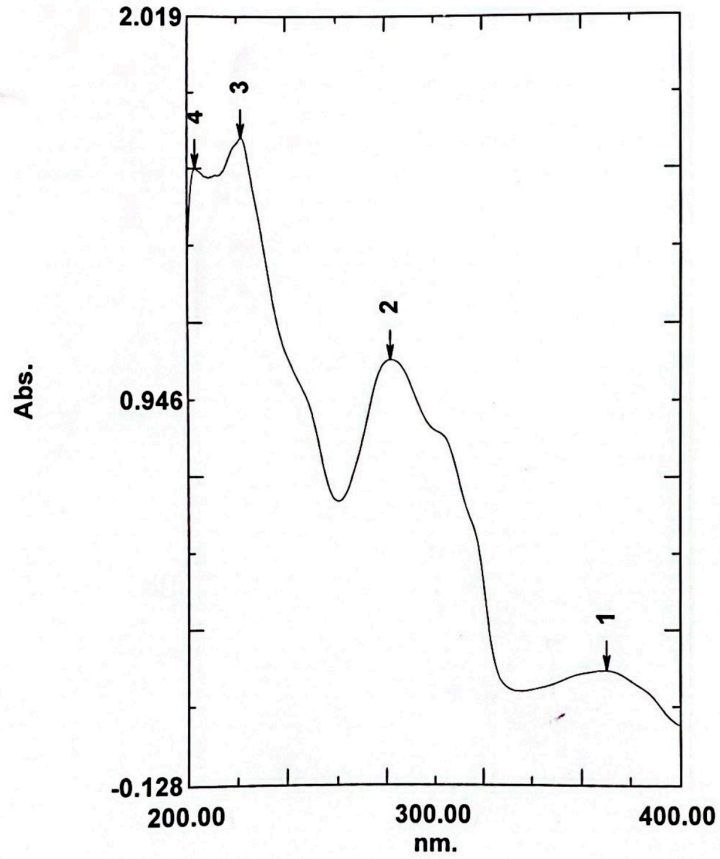

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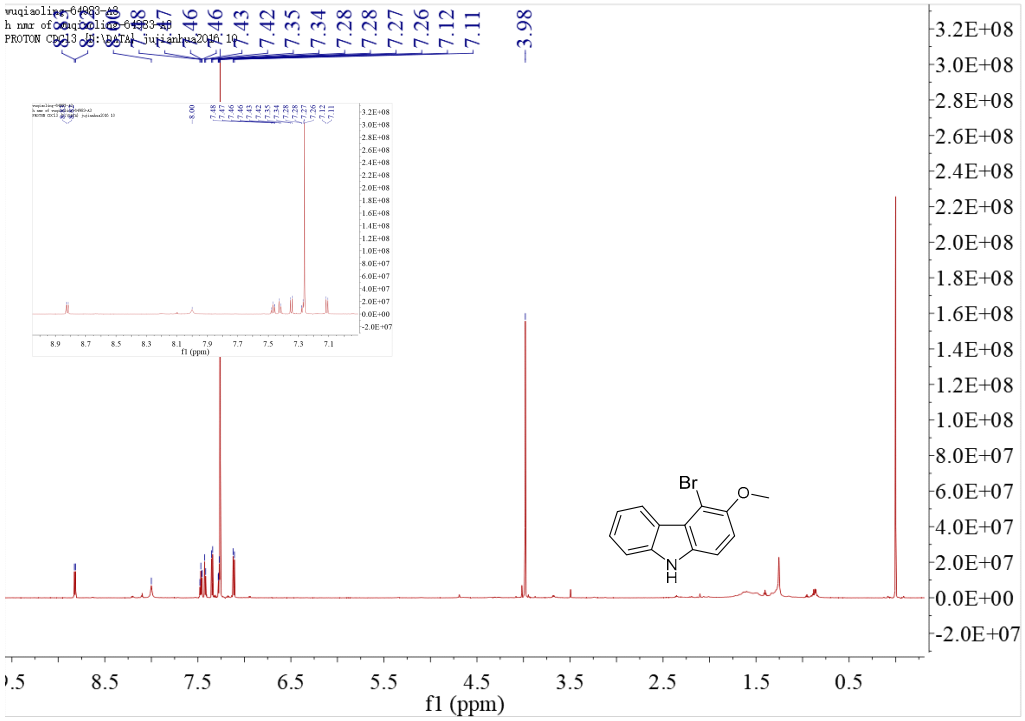

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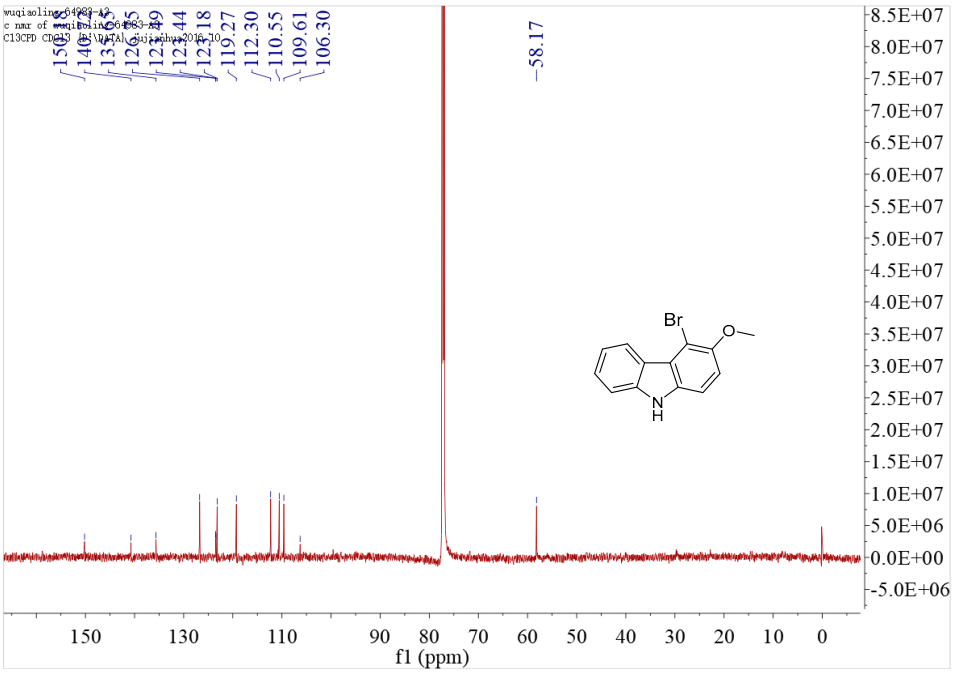

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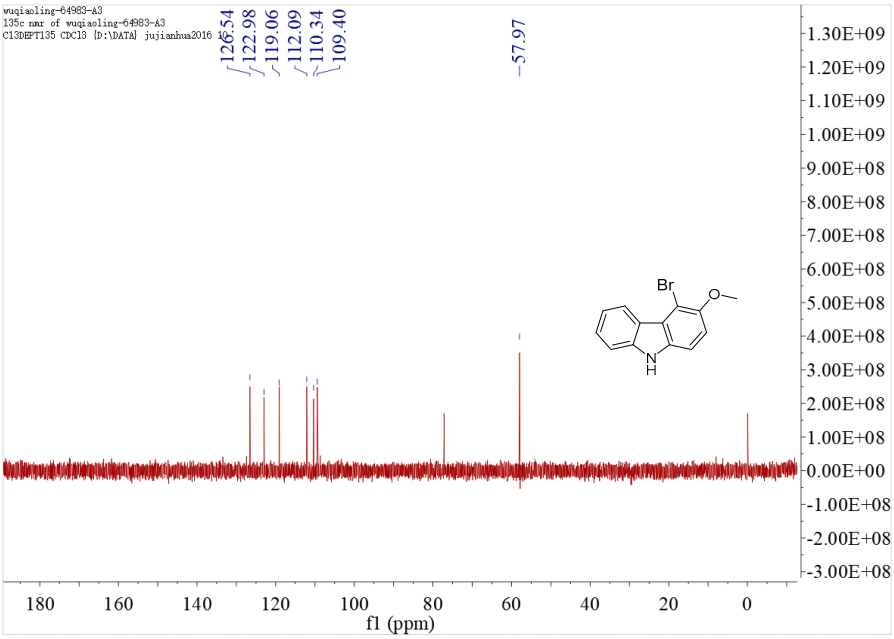

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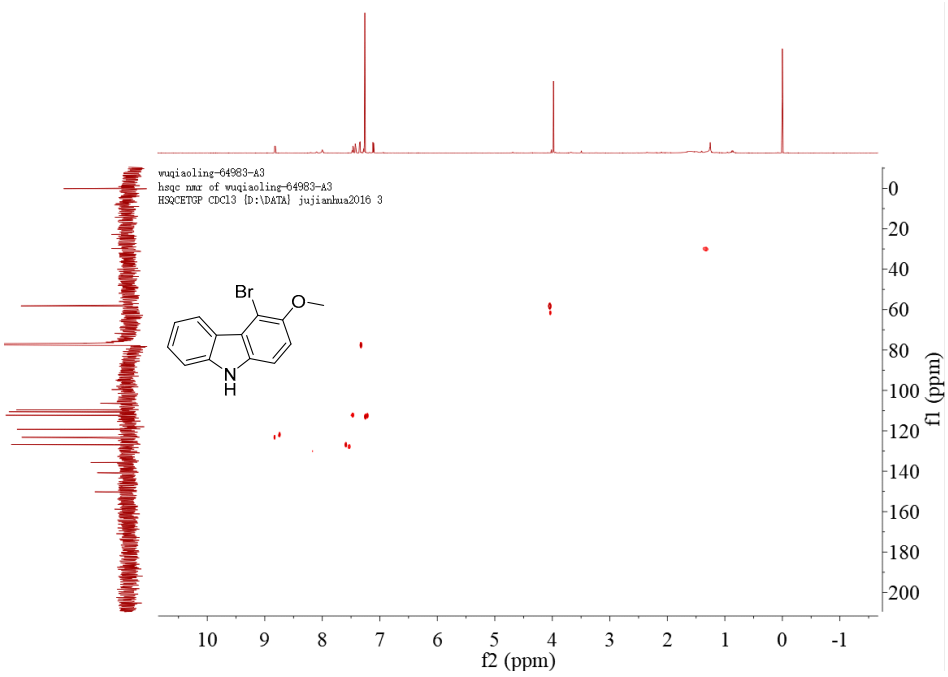
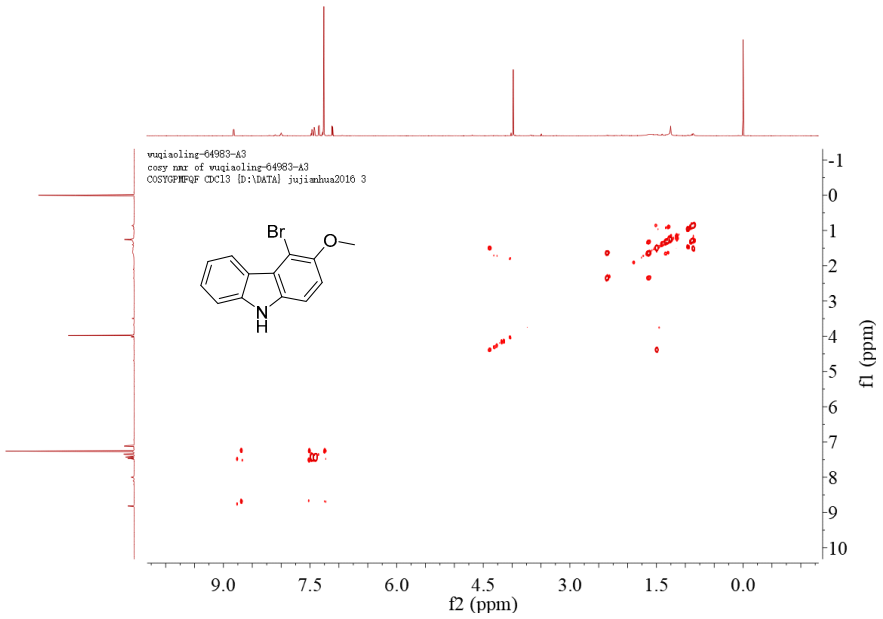


Figure S36. HSQC spectrum of compound **4** in chloroform-*d*.



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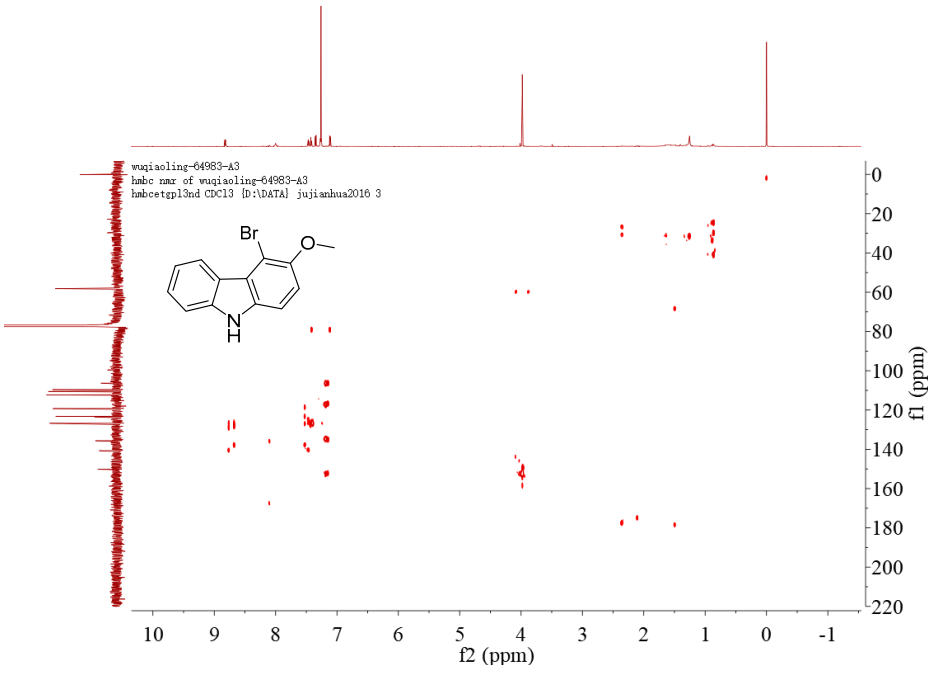

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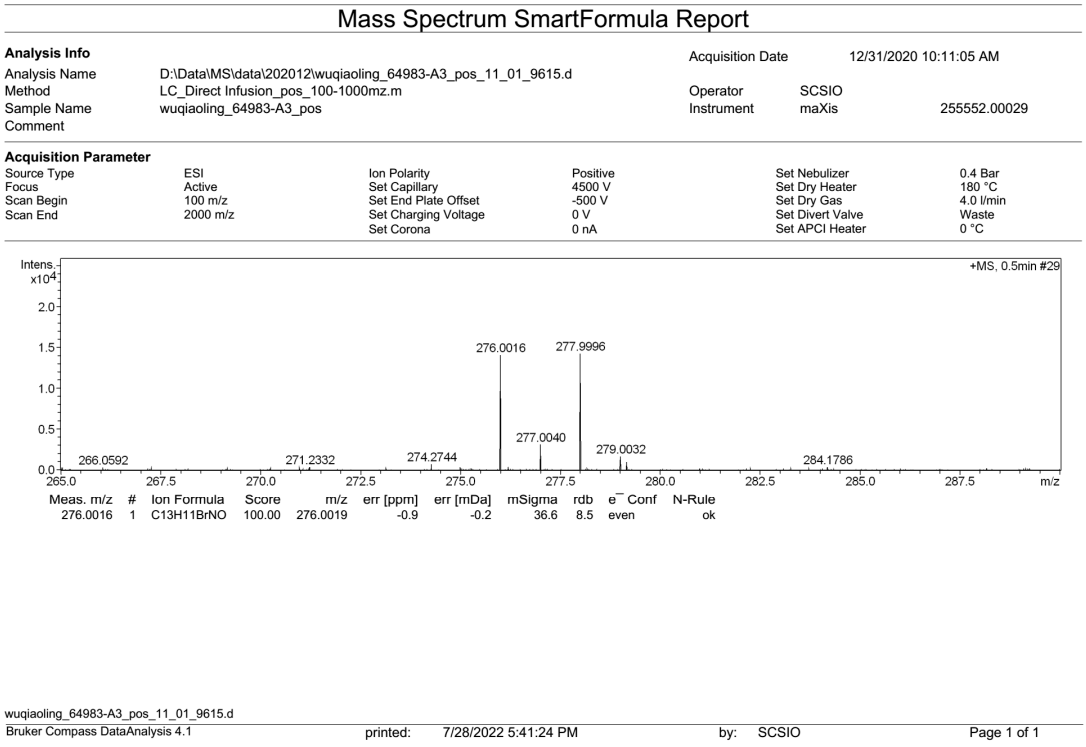

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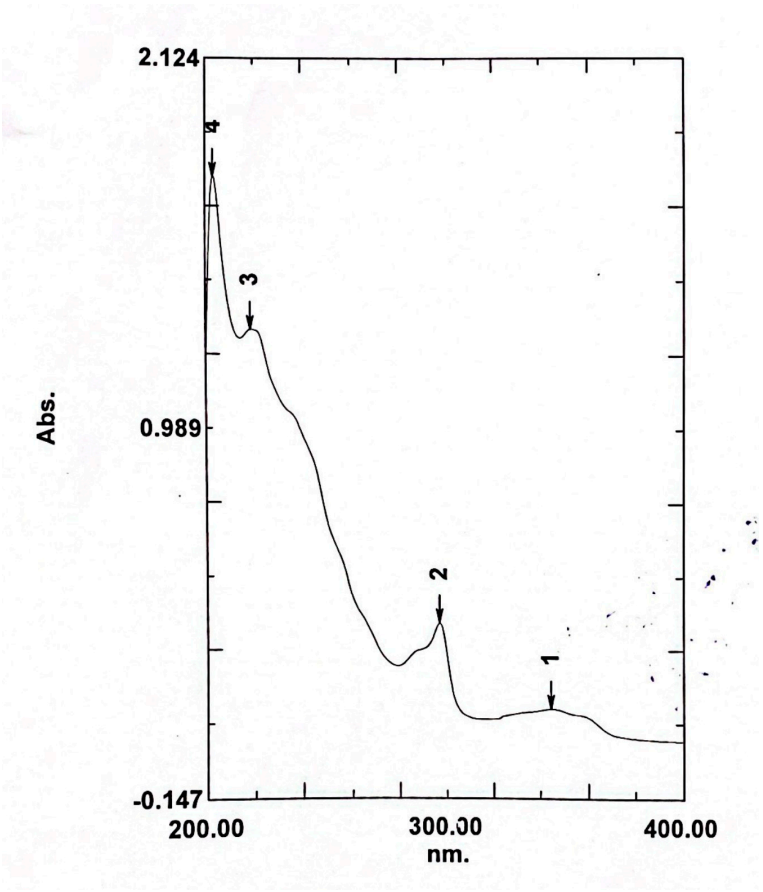

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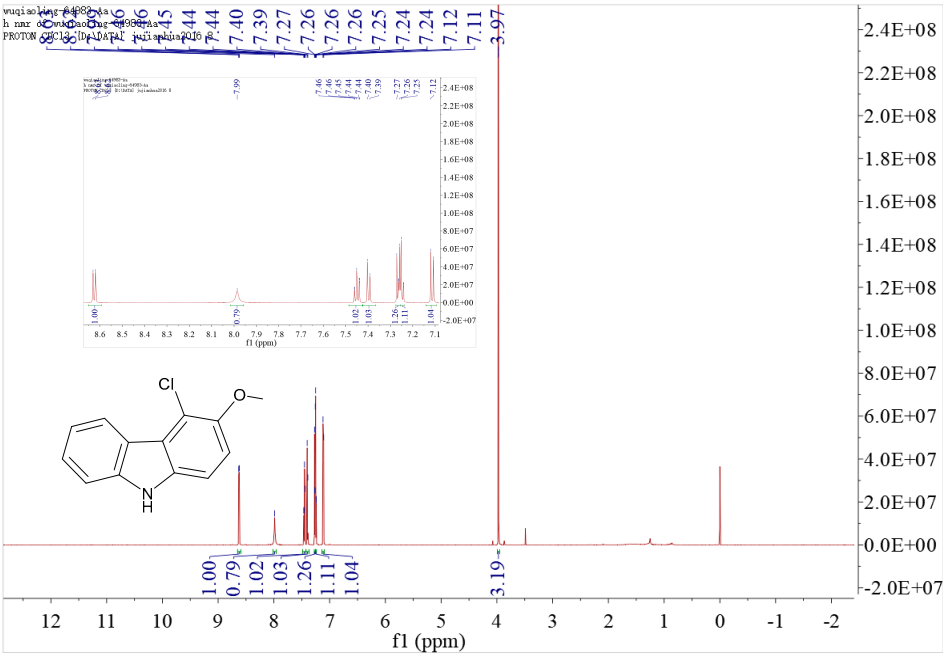

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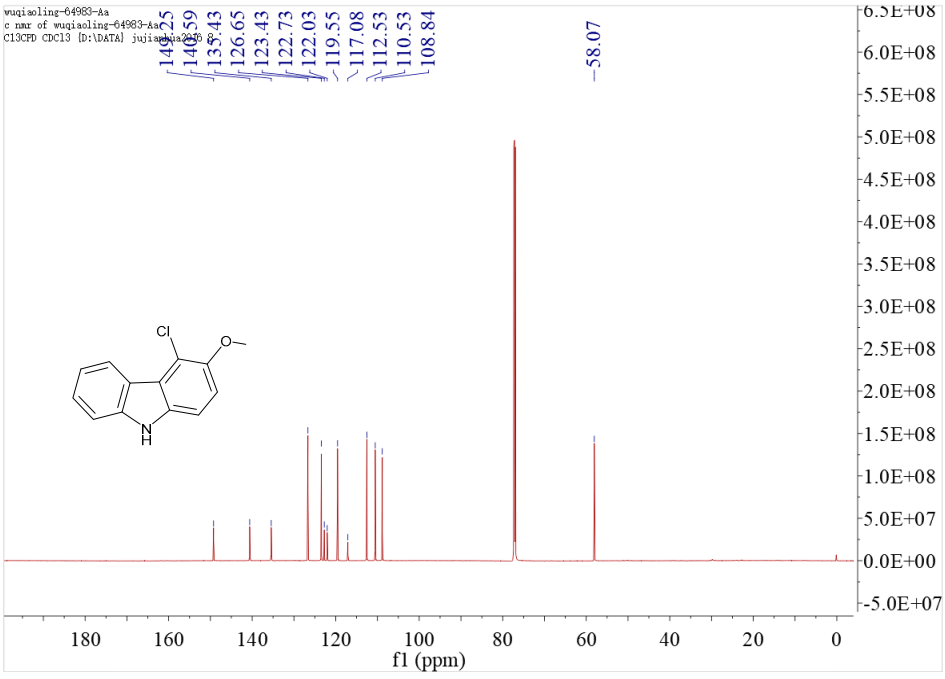

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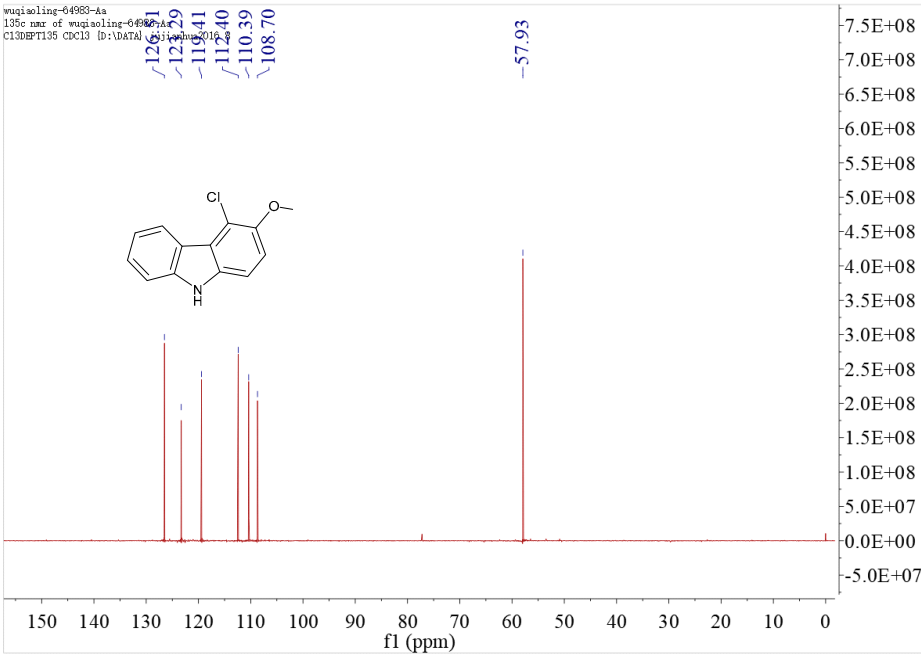

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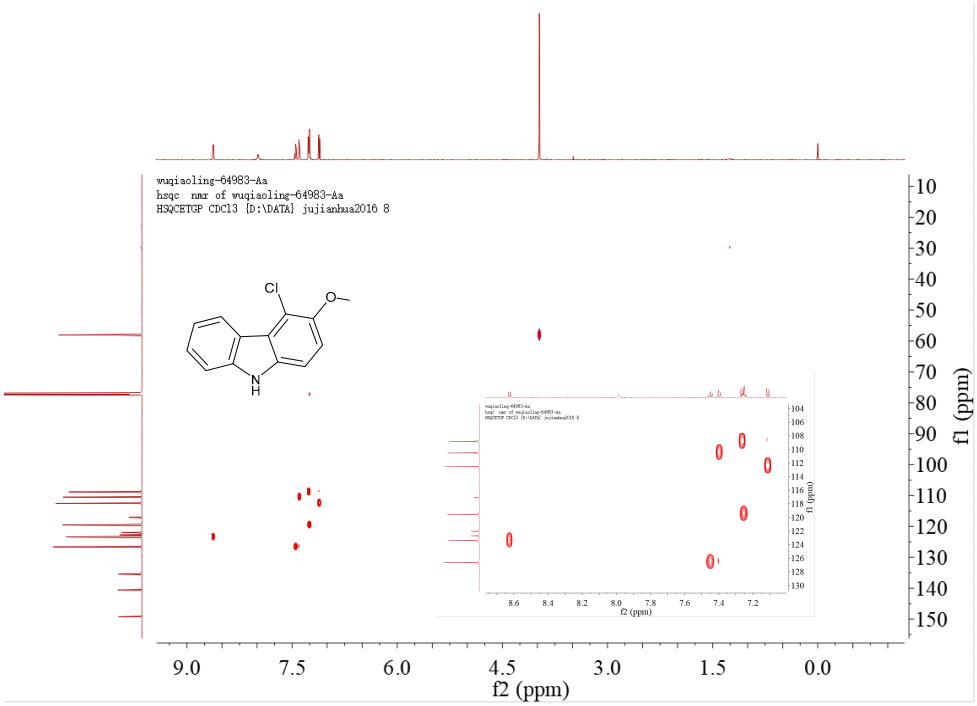

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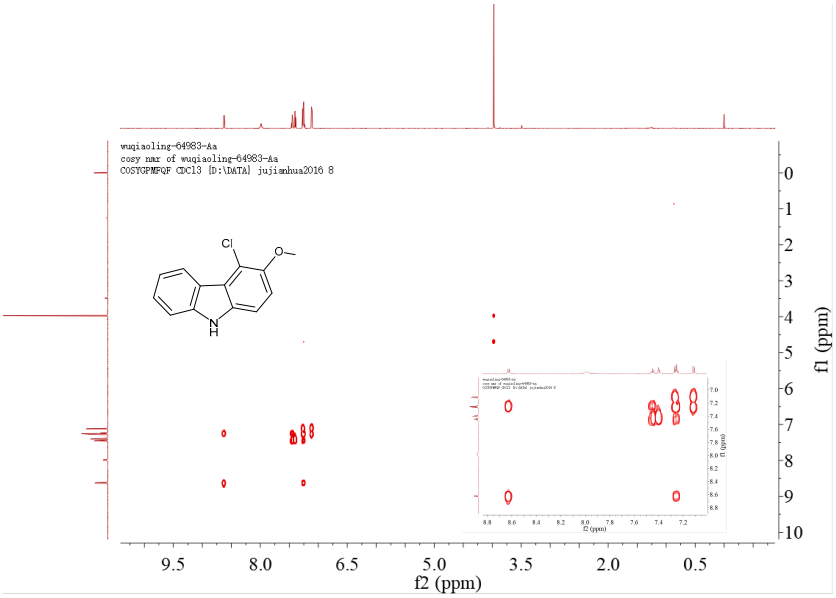
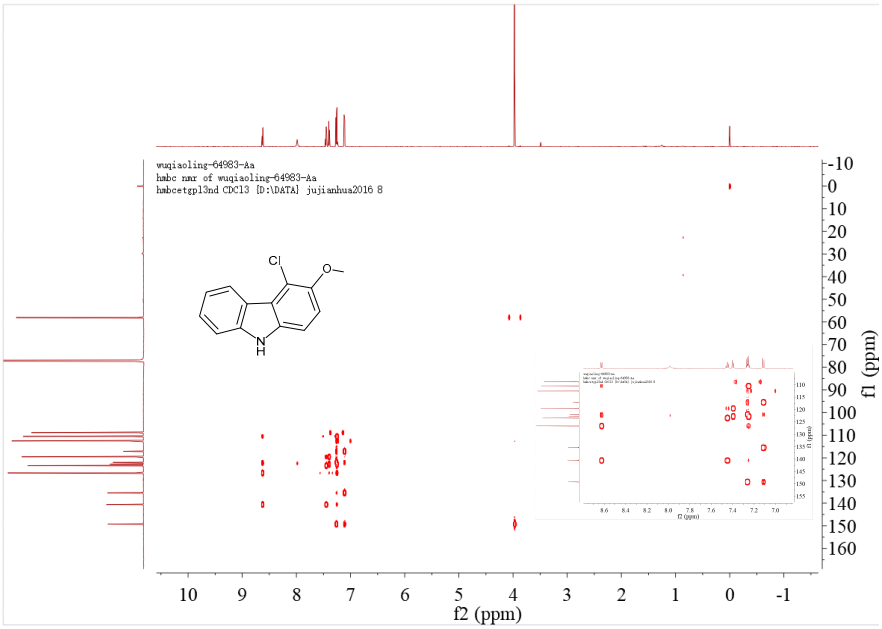


Figure S45. ^{1}H-^{1}H COSY spectrum of compound **5** in chloroform-*d*.



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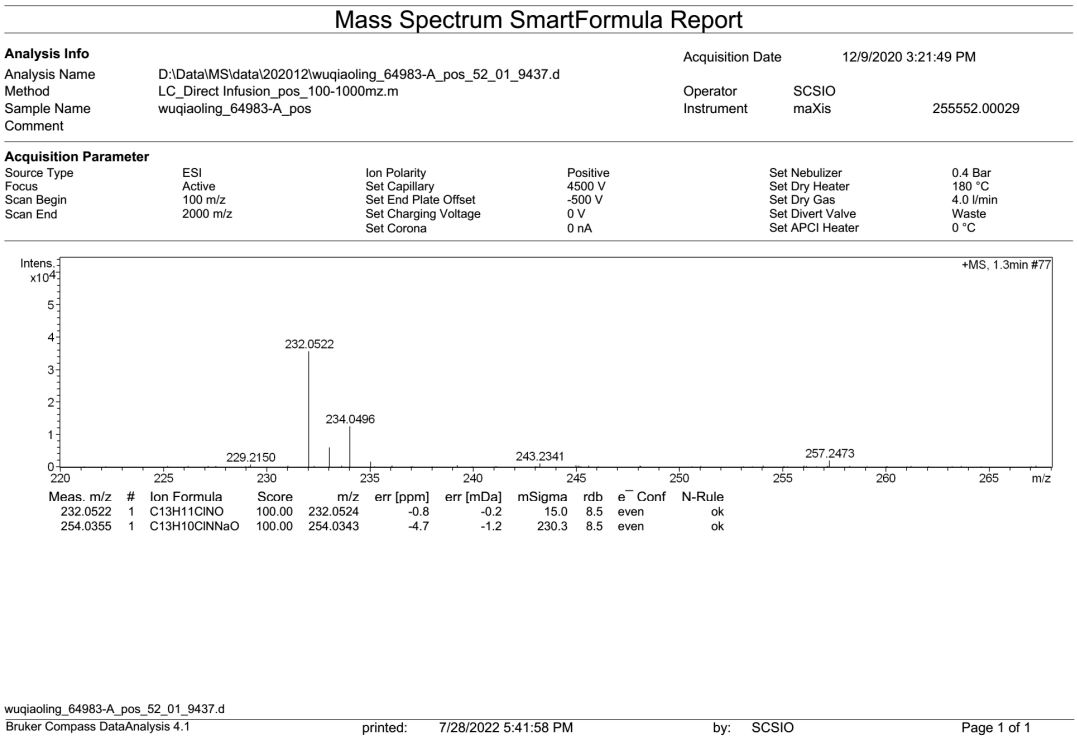
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Comment			

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254.0355	1	C13H10ClNNaO	100.00	254.0343	-4.7	-1.2	230.3	8.5	even	ok

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Figure S47. HRESIMS of compound **5**.

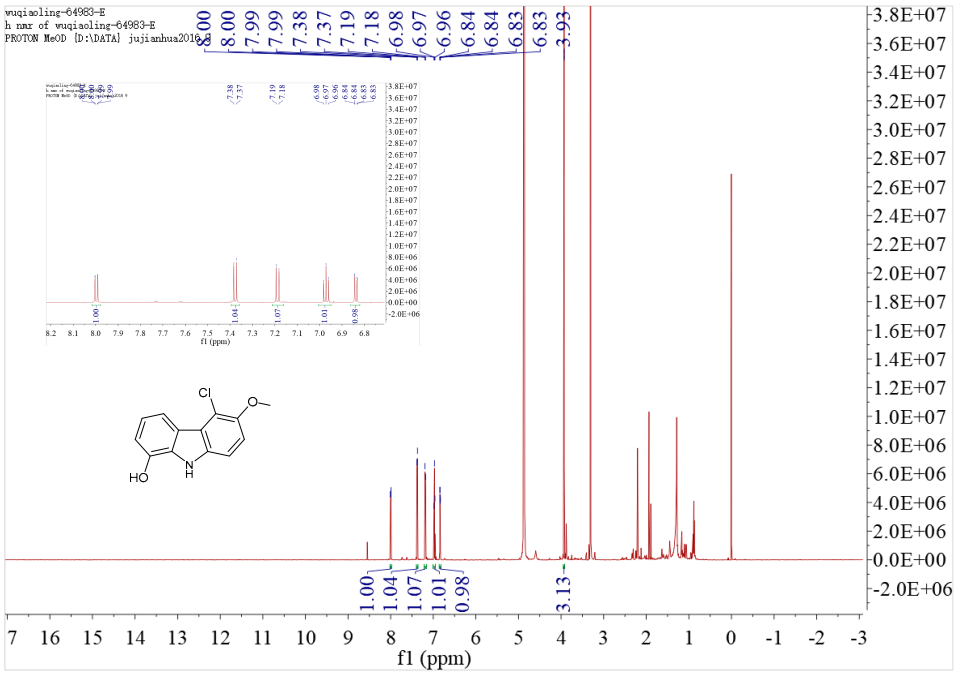

Figure S48. ^{1}H-NMR spectrum of compound **6** in mathanol-d_4.

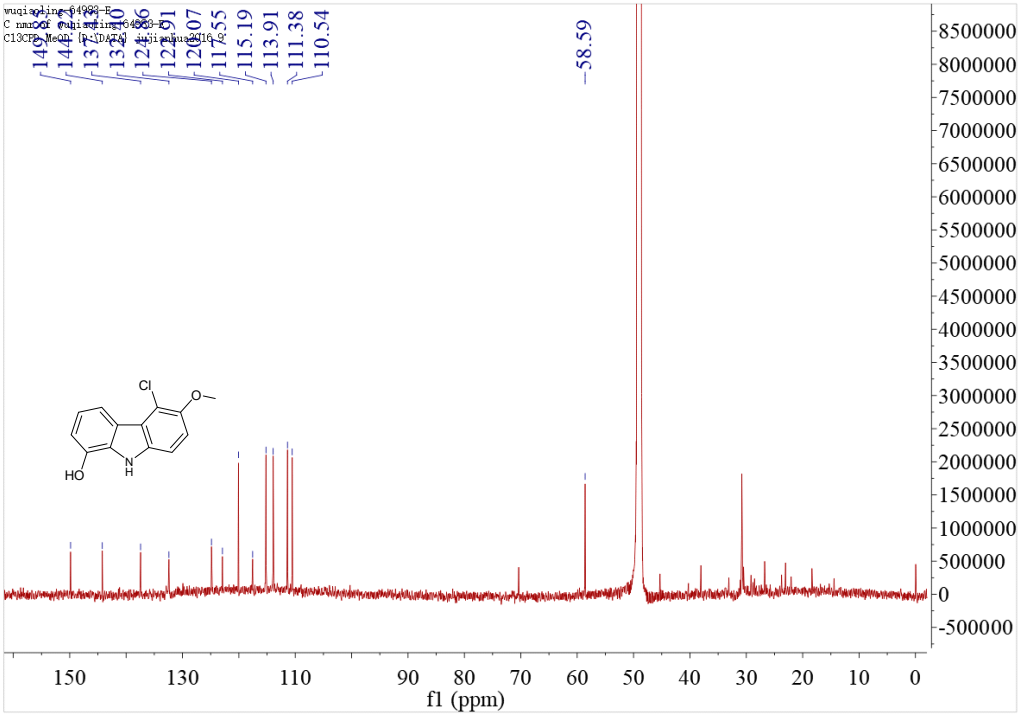

Figure S49.[13]C-NMR spectrum of compound **6** in mathanol-d_4.

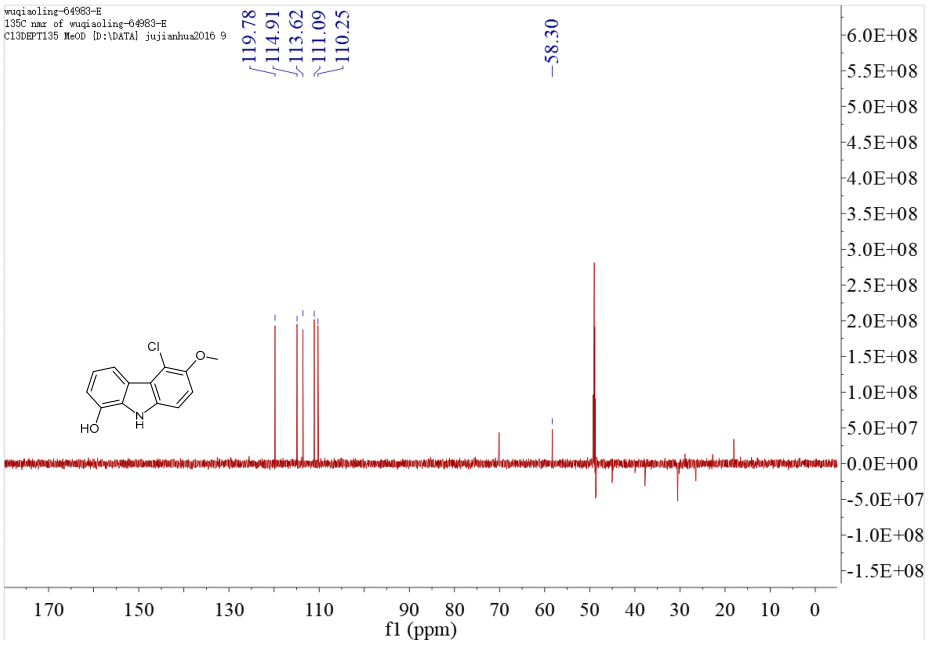

Figure S50. DEPT135 spectrum of compound **6** in mathanol-d_4.

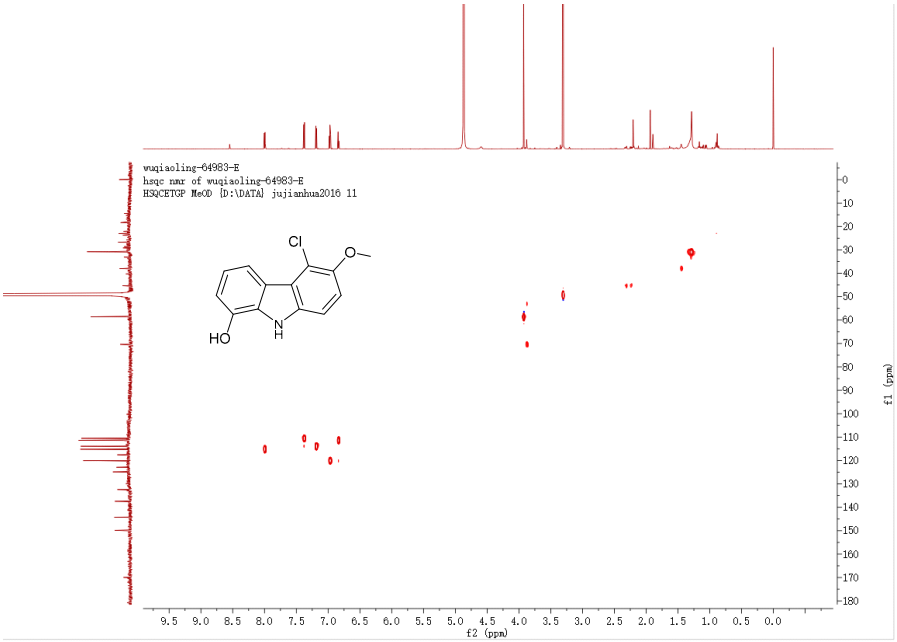

Figure S51. HSQC spectrum of compound **6** in mathanol-d_4.

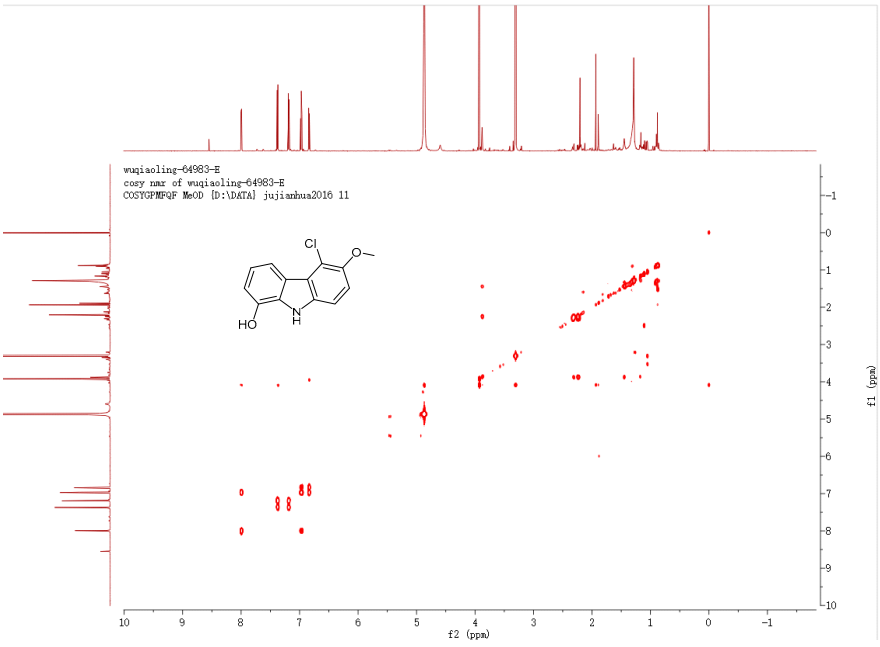

Figure S52. ^{1}H-^{1}H COSY spectrum of compound **6** in mathanol-d_4.

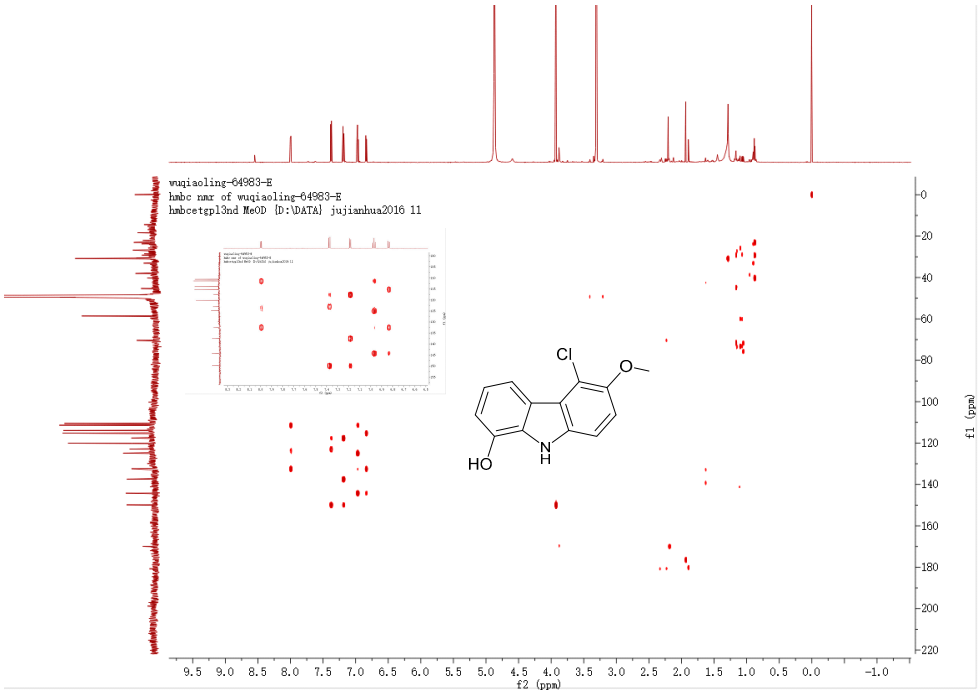

Figure S53. HMBC spectrum of compound **6** in mathanol-d_4.

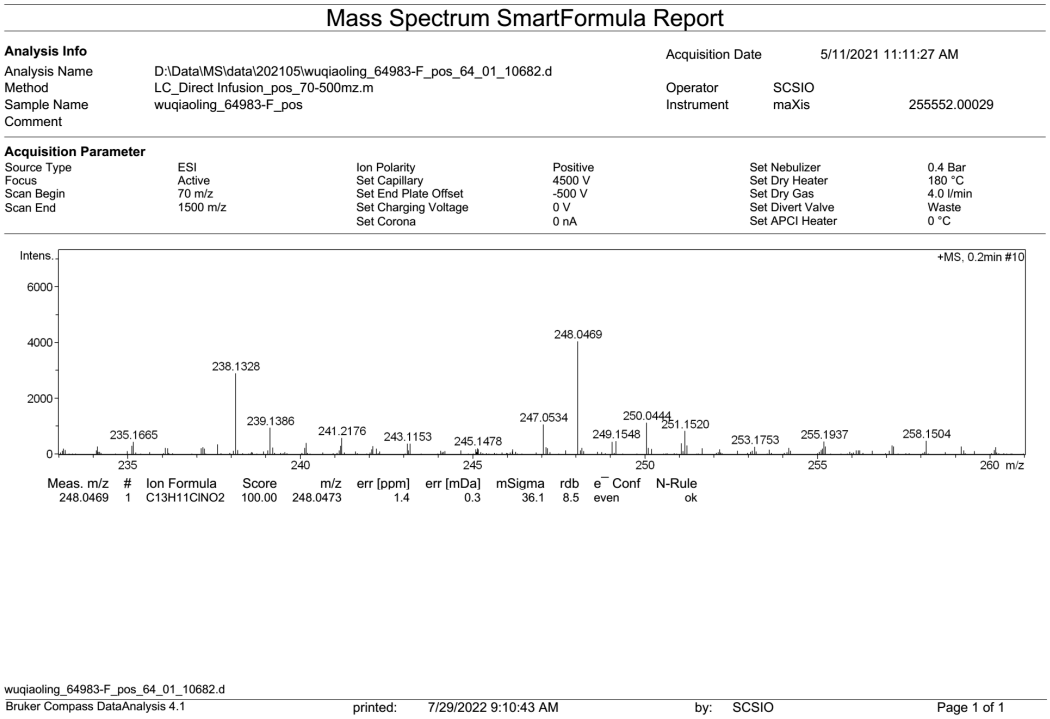

Figure S54. HRESIMS of compound **6**.

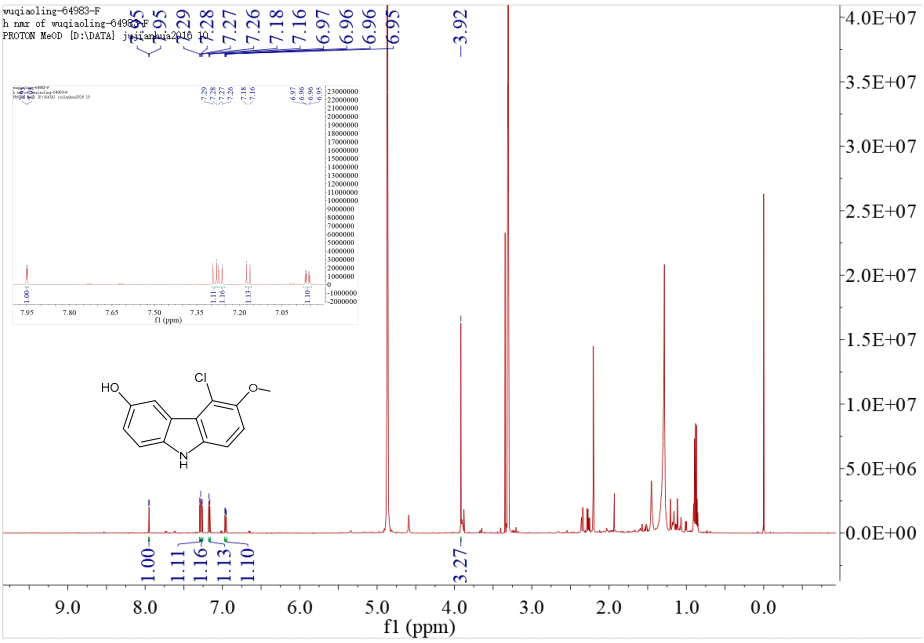

Figure S55.[1]H-NMR spectrum of compound **7** in mathanol-d_4.

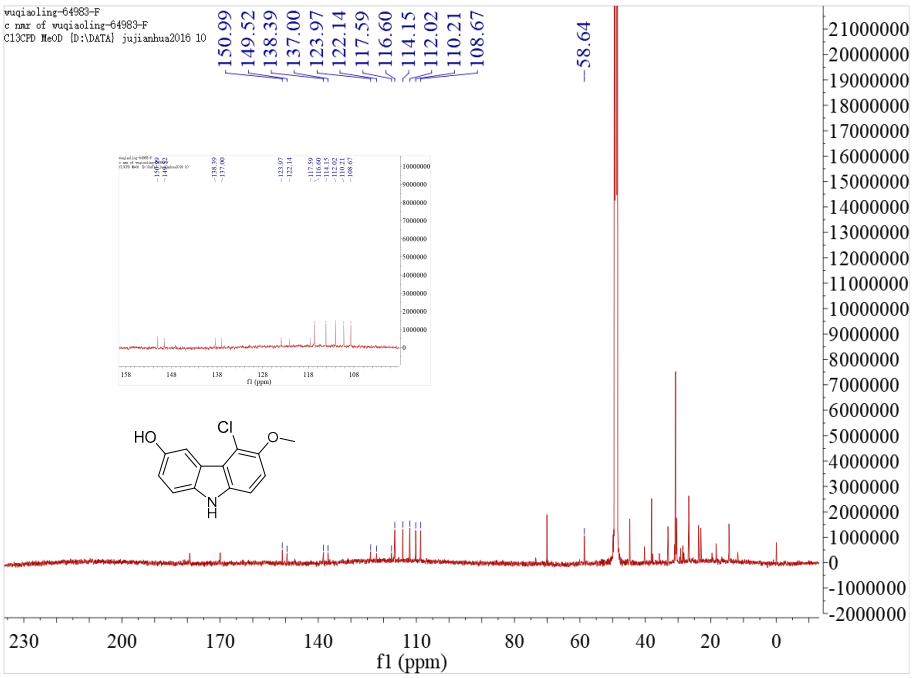

Figure S56.[13]C-NMR spectrum of compound **7** in mathanol-d_4.

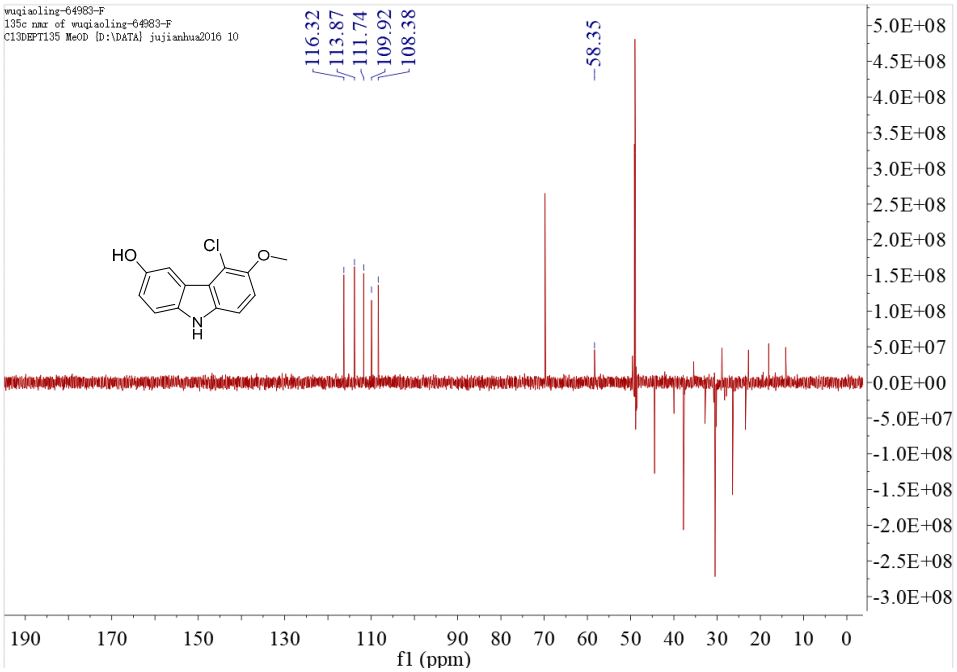

Figure S57. DEPT135 spectrum of compound **7** in mathanol-d_4.

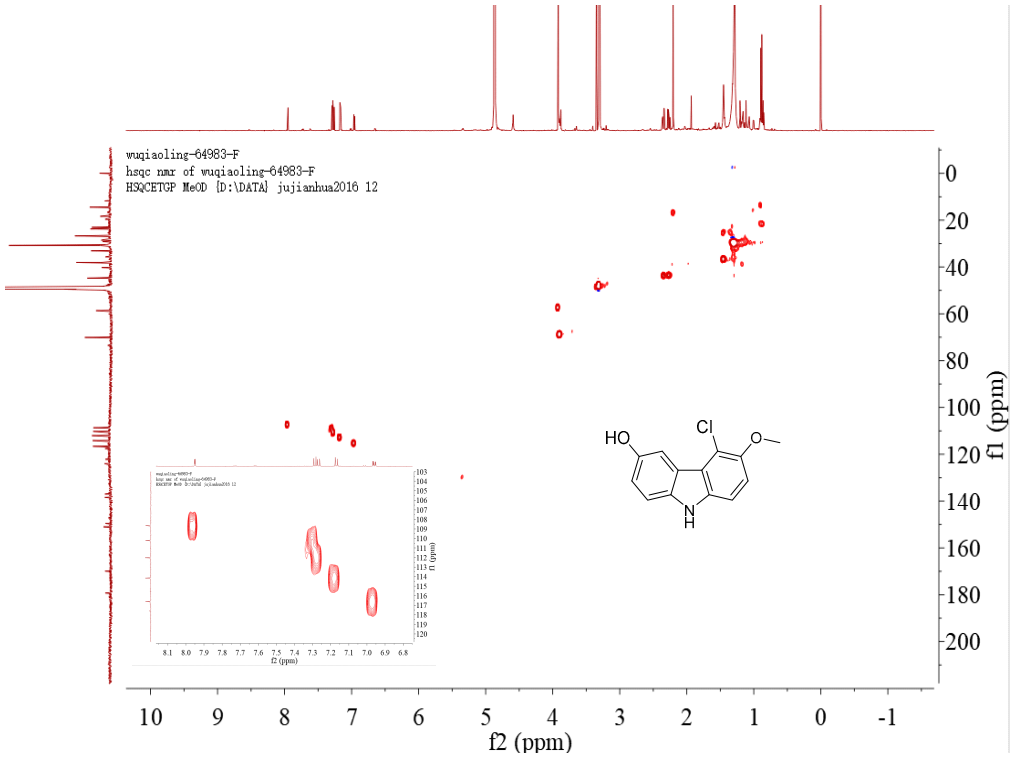

Figure S58. HSQC spectrum of compound **7** in mathanol-d_4.

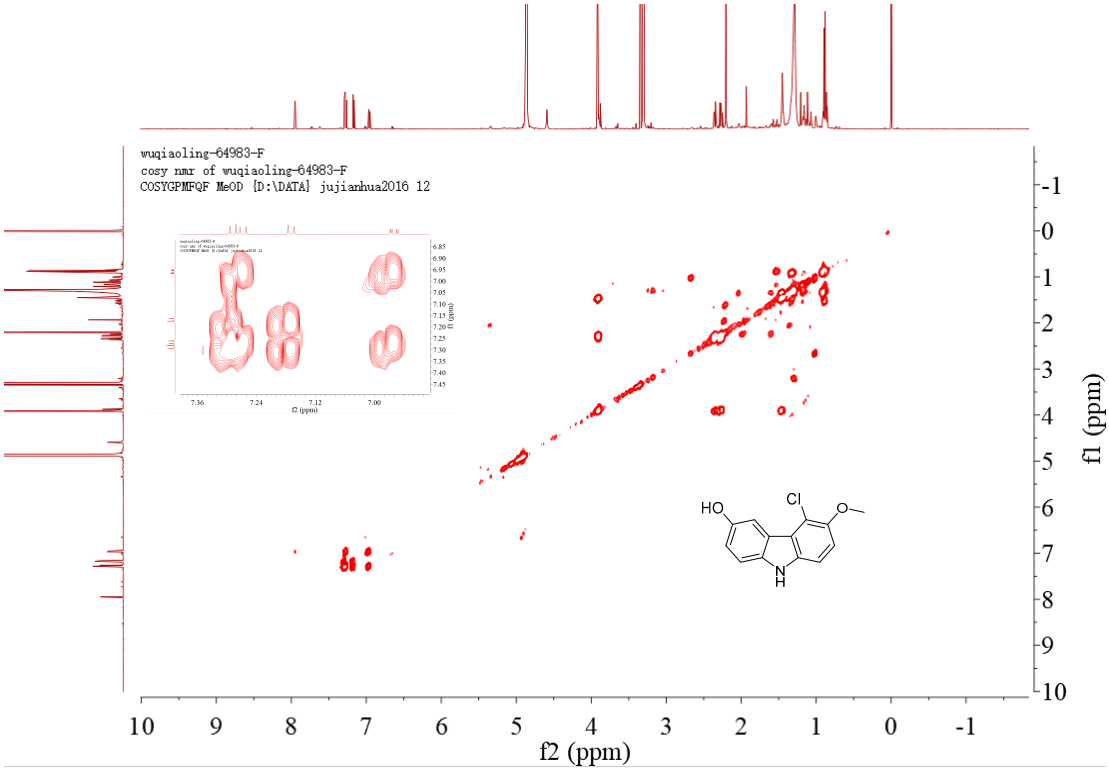

Figure S59.^{1}H-^{1}H COSY spectrum of compound **7** in mathanol-d_4.

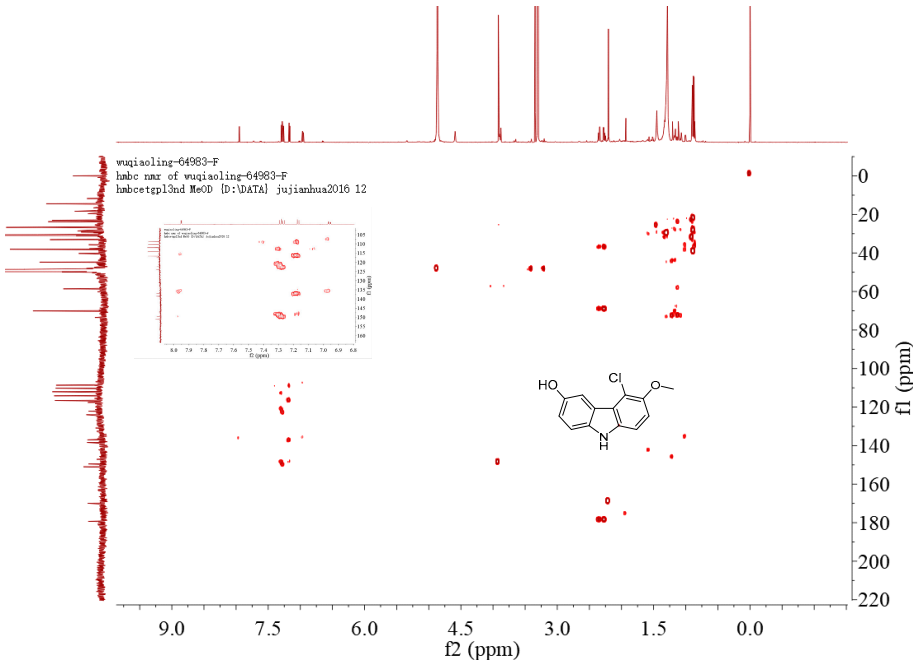

Figure S60. HMBC spectrum of compound **7** in mathanol-d_4.

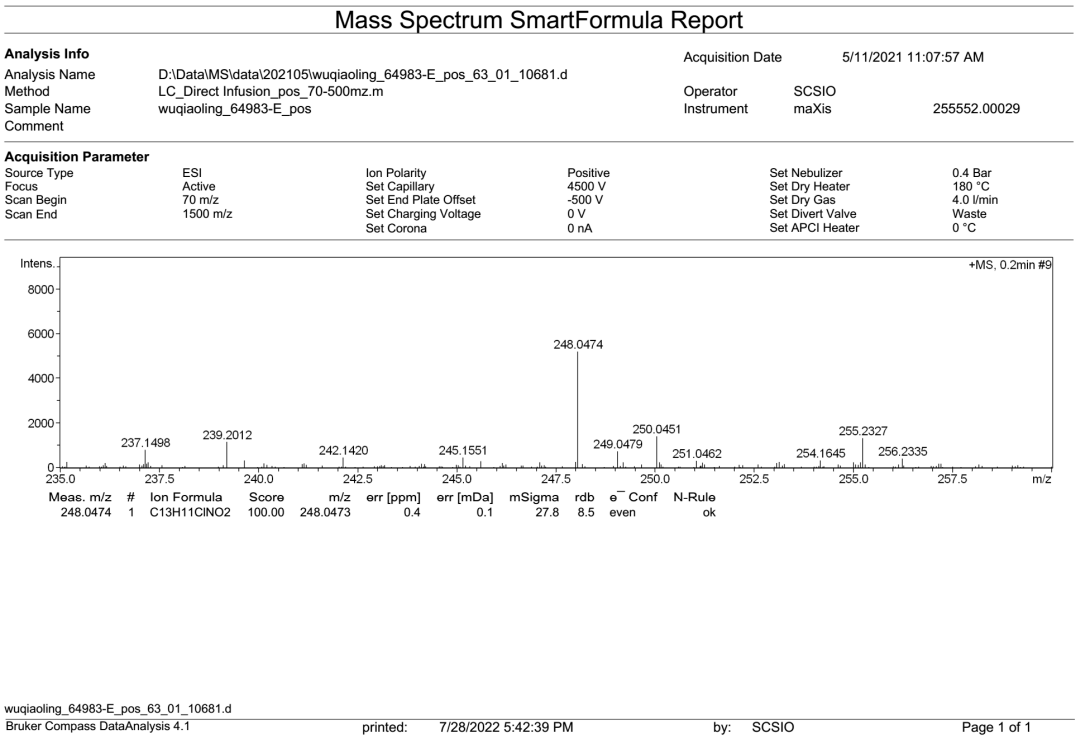

Figure S61. HRESIMS of compound **7**.

2. Medium Formula and Optimization Results of *S. diacarni* SCSIO 64983

In this experiment, 14 kinds of culture media were used for fermentation optimization. The specific medium formula is as follows：

N4: Starch 15 g/L, fish peptone 8 g/L, bacteriological peptone 5 g/L, glycerol 8 g/L, KBr 0.2 g/L, sea salt 30 g/L, calcium carbonate 2 g/L; pH: 7.2-7.4.

M11: Glycerol 30 g/L, Soybean powder 10 g/L, $CaCO_3$ 2 g/L, sea salt 30 g/L; pH: 7.2-7.4.

SCAS: Starch 40 g/L, Acid Hydrolyzed Casein Peptone 5 g/L, KH_2PO_4 0.5 g/L, $MgSO_4{\cdot}7H_2O$ 0.5 g/L, $FeSO_4{\cdot}7H_2O$ 0.5 g/L; pH: 7.2-7.4.

HMT: Glycerol 20 g/L, fish powder 20 g/L, Yeast extract 5 g/L, $CaCO_3$ 5 g/L; pH: 7.2-7.4.

ISP2: Glucose 4 g/L, Yeast extract 4 g/L, Malt extract 10 g/L, sea salt 30 g/L; pH: 7.2-7.4.

ISP3: Oatmeal 20 g/L, Trace elements 1mL/L, $FeSO_4{\cdot}7H_2O$ 0.1 g/L, $MnCL_2{\cdot}4H_2O$:0.1 g/L, $ZnSO_4.7H_2O$ 0.1 g/L; pH: 7.2-7.4.

ISP4: Starch 10 g/L, Bacteriological Peptone 1 g/L, Yeast extract 5 g/L, KH_2PO_4 1 g/L, $MgSO_4{\cdot}7H_2O$ 1 g/L, NaCl 1 g/L, $(NH_4)_2SO_4$ 2 g/L, sea salt 30 g/L, $CaCO_3$ 2 g/L, Trace elements 1mL/L; pH: 7.2-7.4.

AM2ab: Starch 15 g/L, Soybean powder 5 g/L, sea salt 30 g/L, Glucose 20 g/L, $MgSO_4{\cdot}7H_2O$ 0.5 g/L, $CaCO_3$ 2 g/L, Yeast extract 2 g/L, KH_2PO_4 0.5 g/L, Bacteriological Peptone 2 g/L, NaCl 4 g/L; pH: 7.2-7.4.

RA: Glucose 10 g/L, Starch 20 g/L, Malt extract 10 g/L, sea salt 30 g/L, corn powder 5 g/L, maltose 10 g/L, $CaCO_3$ 2 g/L, Trace elements 100 μL; pH: 7.2-7.4.

AM3: Starch 15 g/L, Soybean powder 10 g/L, glycerol 15 g/L, Bacteriological Peptone 15 g/L, sea salt 30 g/L, $CaCO_3$ 5 g/L; pH: 7.2-7.4.

LB: TRYPTONE 10g/L, Yeast extract 5g/L, NaCl 10g/L; pH: 7.2-7.4.
YMS: Yeast extract 4g/L, Malt extract 10g/L, Starch 4 g/L, Oatmeal 8 g/L, sea salt 30 g/L; pH: 7.2-7.4.
MS: Soybean powder 20 g/L, Mannitol 20 g/L; pH: 7.2-7.4.
TSB: TSB finished powder 30 g/L; pH: 7.2-7.4.

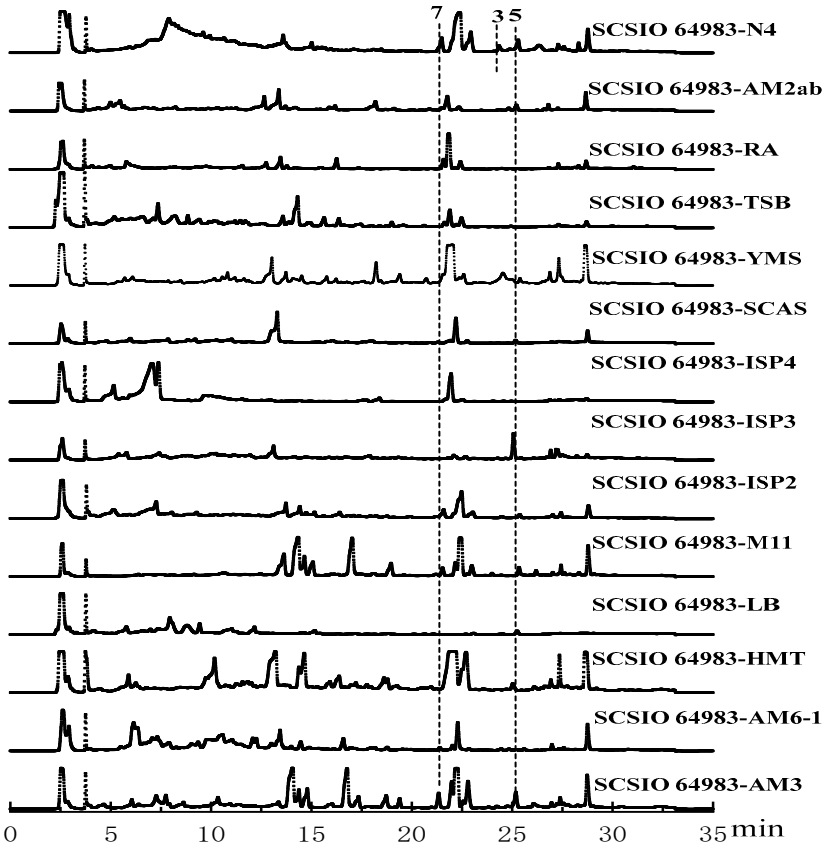

Figure S62. Optimization Results of *S. diacarni* SCSIO 64983

3. NMR data of **6**-**7** in methanol-d_4 and **1**–**2** in DMSO-d_6

Table S1. NMR data of **6**-**7** in methanol-d_4 and **1**–**2** in DMSO-d_6

Position	6[a]		7[a]		1[C]		2[C]	
	δ_C, type	**δ_H (J in Hz)**	**δ_C, type**	**δ_H (J in Hz)**	**δ_C, type**	**δ_H (J in Hz)**	**δ_C, type**	**δ_H (J in Hz)**
1	110.5, CH	7.38, d (8.7)	110.1, CH	7.29, d (8.7)	111.0, CH	7.49, d (8.1)	110.1, CH	7.42, d (8.7)
2	113.9, CH	7.19, d (8.7)	114.1, CH	7.17, d (8.7)	125.6, CH	7.40, m	113.5, CH	7.32, d (8.7)
3	149.9, C	-	149.5, C	-	118.5, CH	7.18, t (7.5)	148.6, C	-
4	117.6, C	-	117.6, C	-	122.0, CH	8.28, d (7.9)	113.6, C	-
4a	123.0, C	-	122.0, C	-	121.9, C	-	120.3, C	-
4b	124.8, C	-	123.8, C	-	118.8, C	-	118.5, C	-
5	115.2, CH	8.00, dd (0.7,8.0)	108.6, CH	7.95, d (2.4)	112.6, C	-	115.1, C	-
6	120.1, CH	6.97, t (7.8)	150.9, C	-	129.9, C	-	130.1, C	-
7	111.4, CH	6.84, dd (0.7,7.6)	116.6, CH	6.95, dd (2.4,8.6)	115.9, CH	7.08, d (8.5)	118.1, CH	7.16, d (8.5)
8	144.2, C	-	112.0, CH	7.27, d (8.6)	109.2, CH	7.33, d (8.5)	109.7, CH	7.34, d (8.5)
8a	132.5, C	-	136.9, C	-	135.9, C	-	137.6, C	-
9a	137.5, C	-	138.3, C	-	140.2, C	-	136.5, C	-
1''	-	-	-	-	164.3, C	-	165.8, C	-
2''	-	-	-	-	29.0, CH_2	3.59, s	30.4, CH_2	3.30, s
3-OMe	58.6, CH_3	3.93, s	58.6, CH_3	3.92, s	-	-	57.6, CH_3	3.87, s
6-OMe	-	-	-	-	-	-	-	-
9-NH	-	-	-	-	-	11.37	-	11.59
10-NH	-	-	-	-	-	10.52	-	10.37

[a] The data were recorded in methanol-d_4; [b] The data were recorded in chloroform-d; [C] The data were recorded in DMSO-d_6.