Supporting Information

A NEW PHENOLIC COMPOUND FROM SALIX GLANDULOSA

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Figure S1. HRESIMS spectrum of **1**

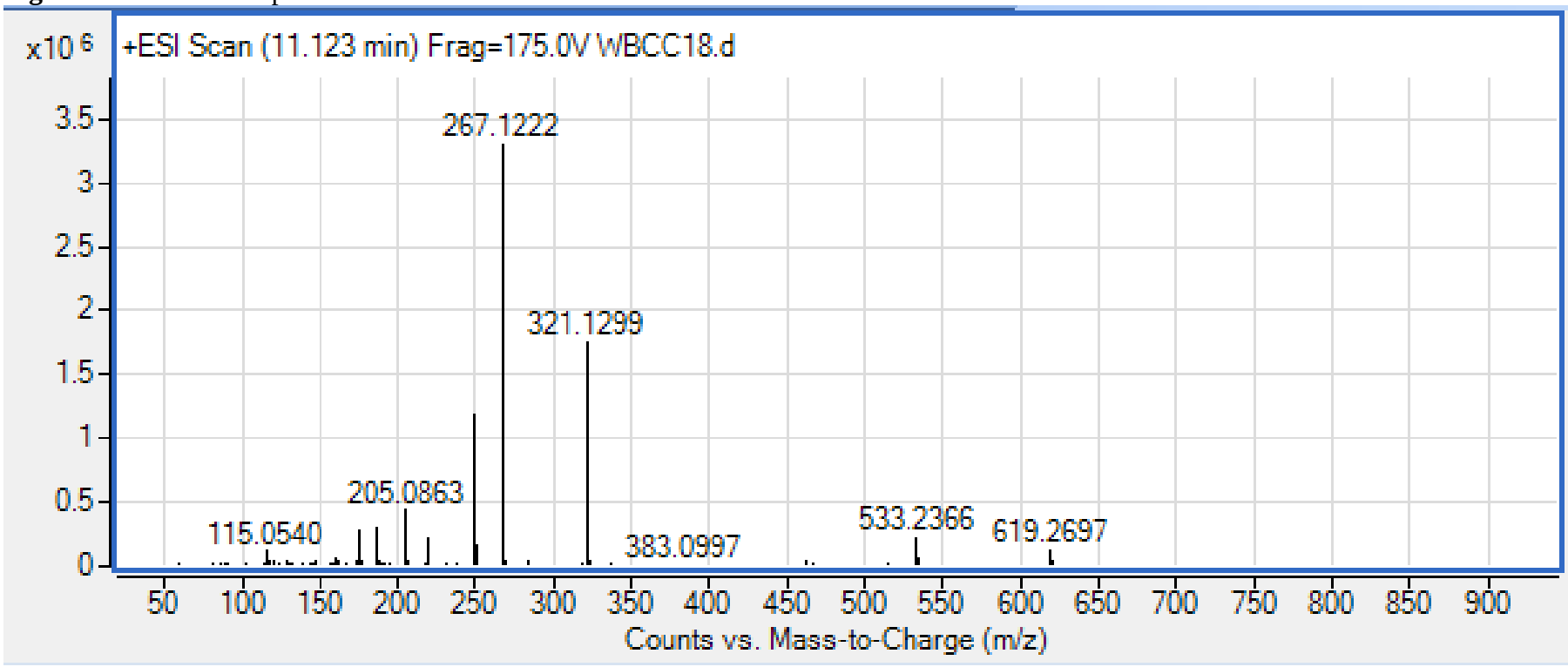


Figure S2. ^{1}H NMR spectrum of **1**

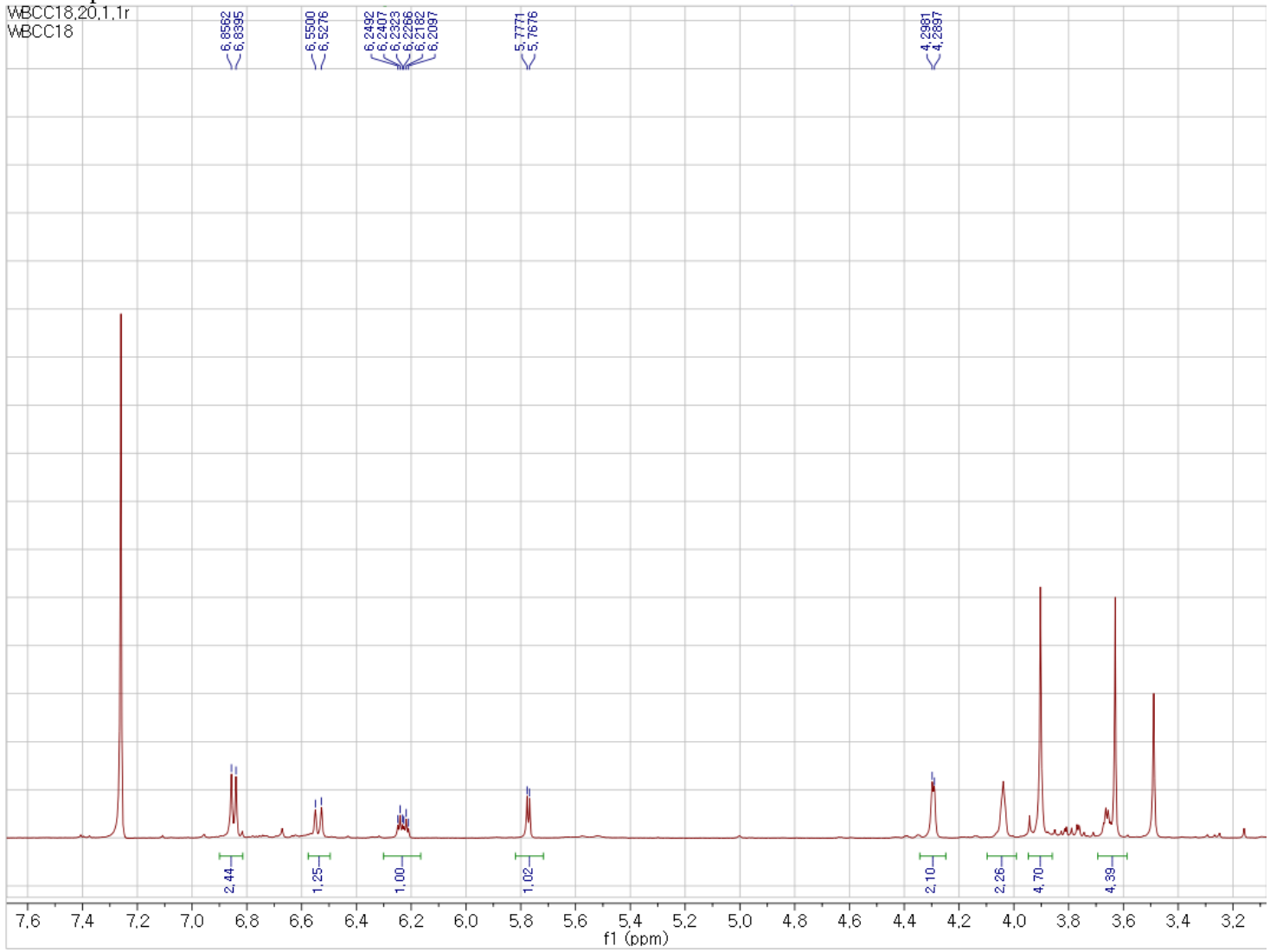


Figure S3. ^{13}C NMR spectrum of **1**

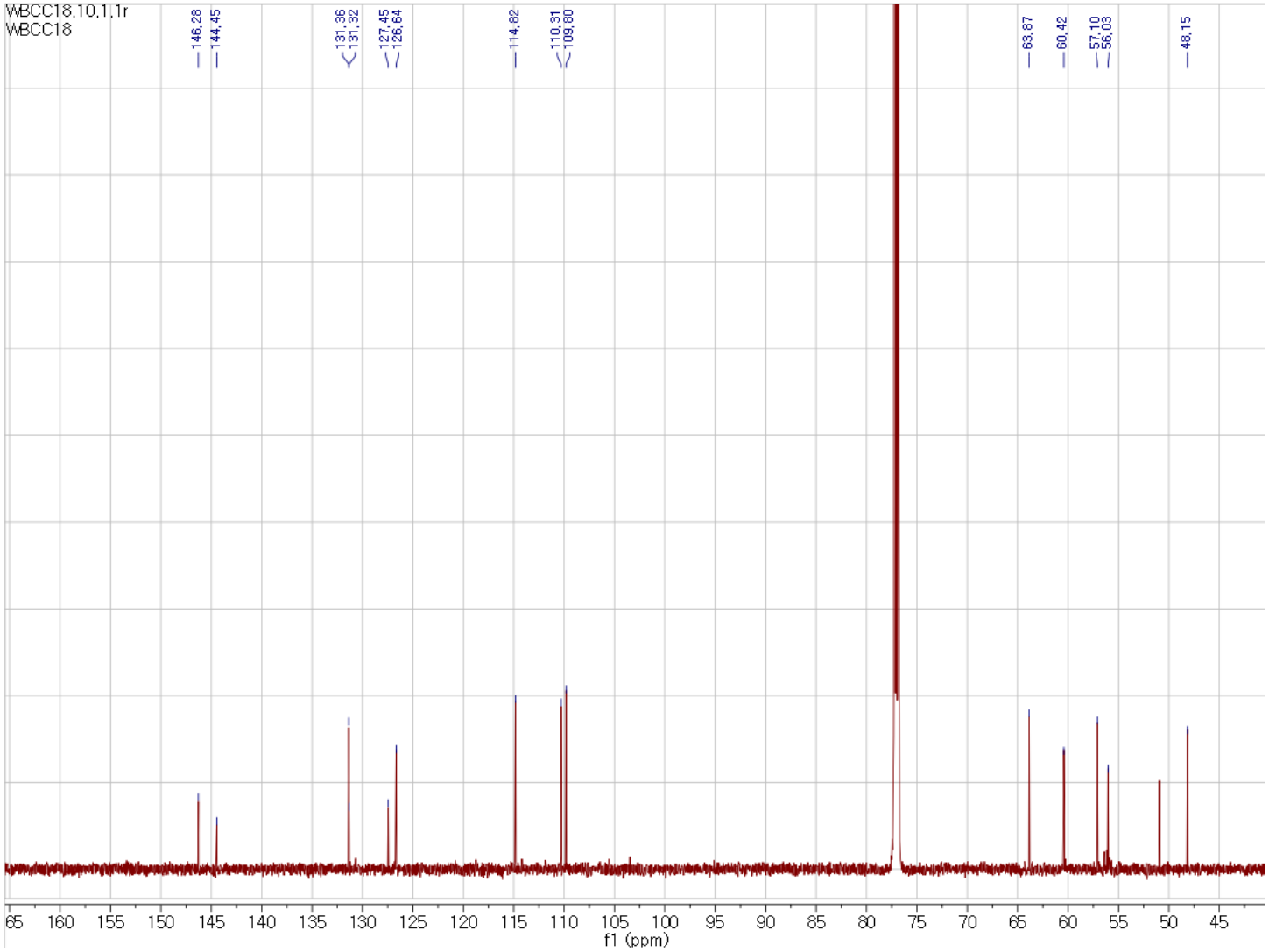


Figure S4. HSQC spectrum of **1**

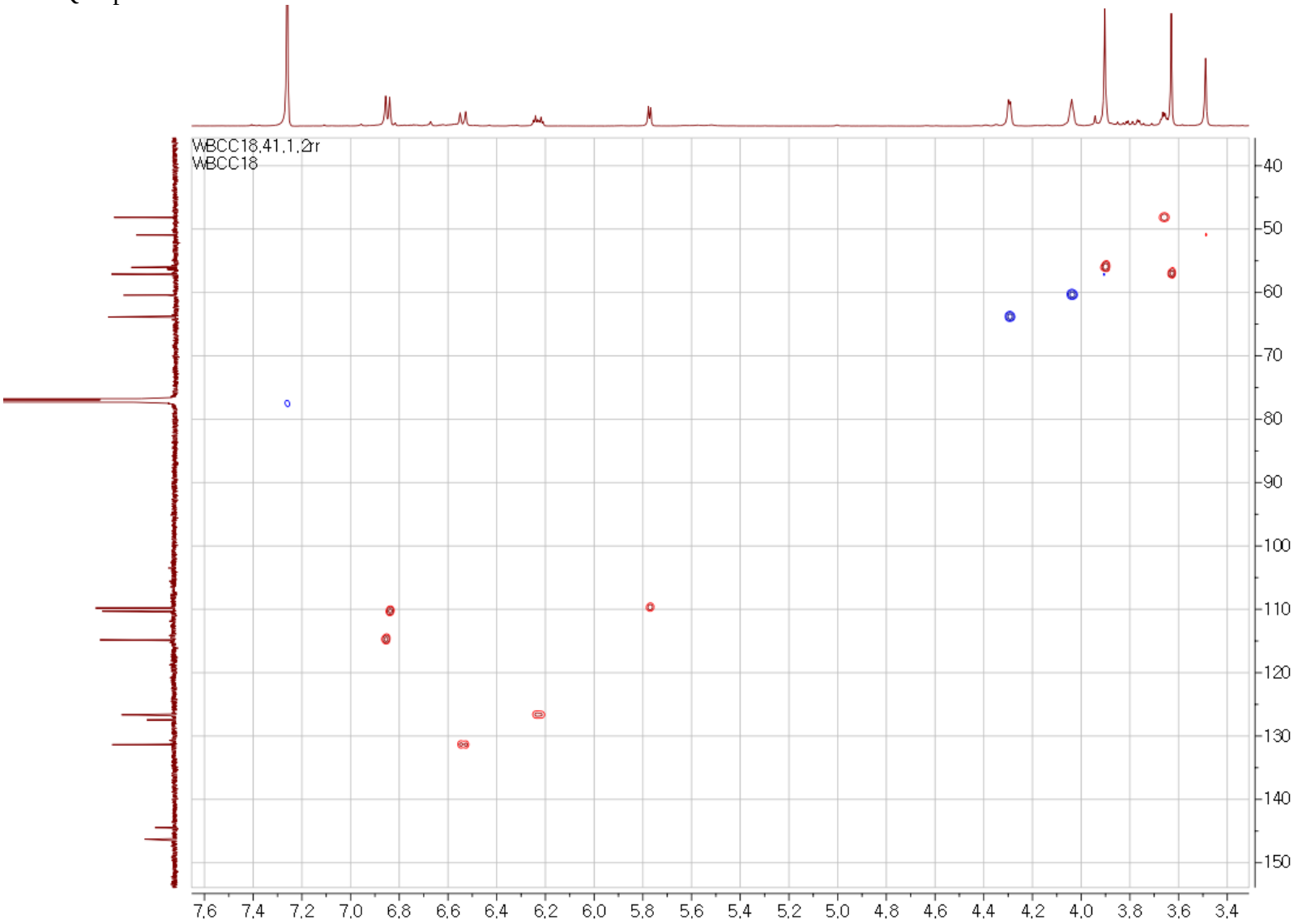


Figure S5. HMBC spectrum of **1**

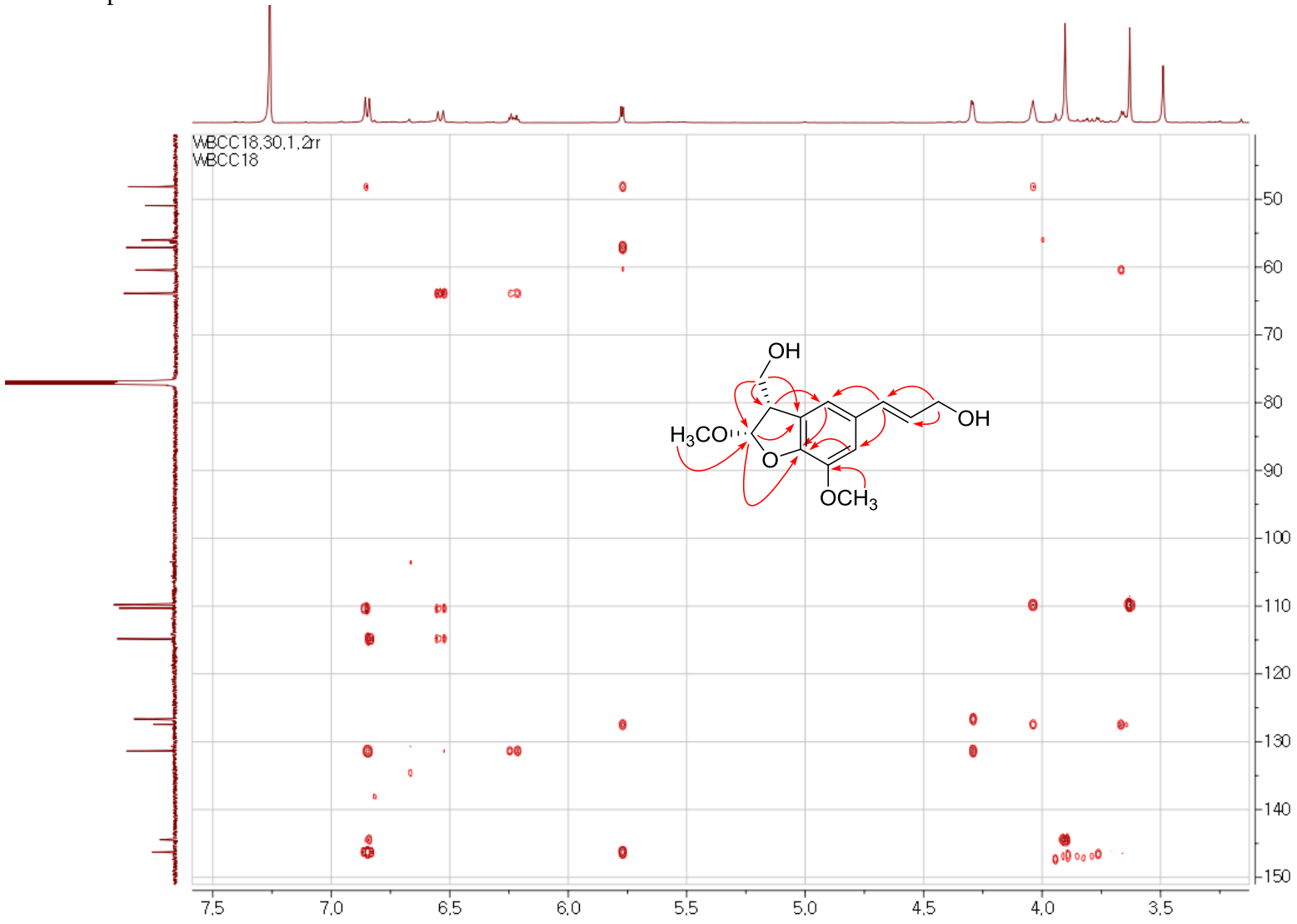


Figure S6. NOESY spectrum of **1**

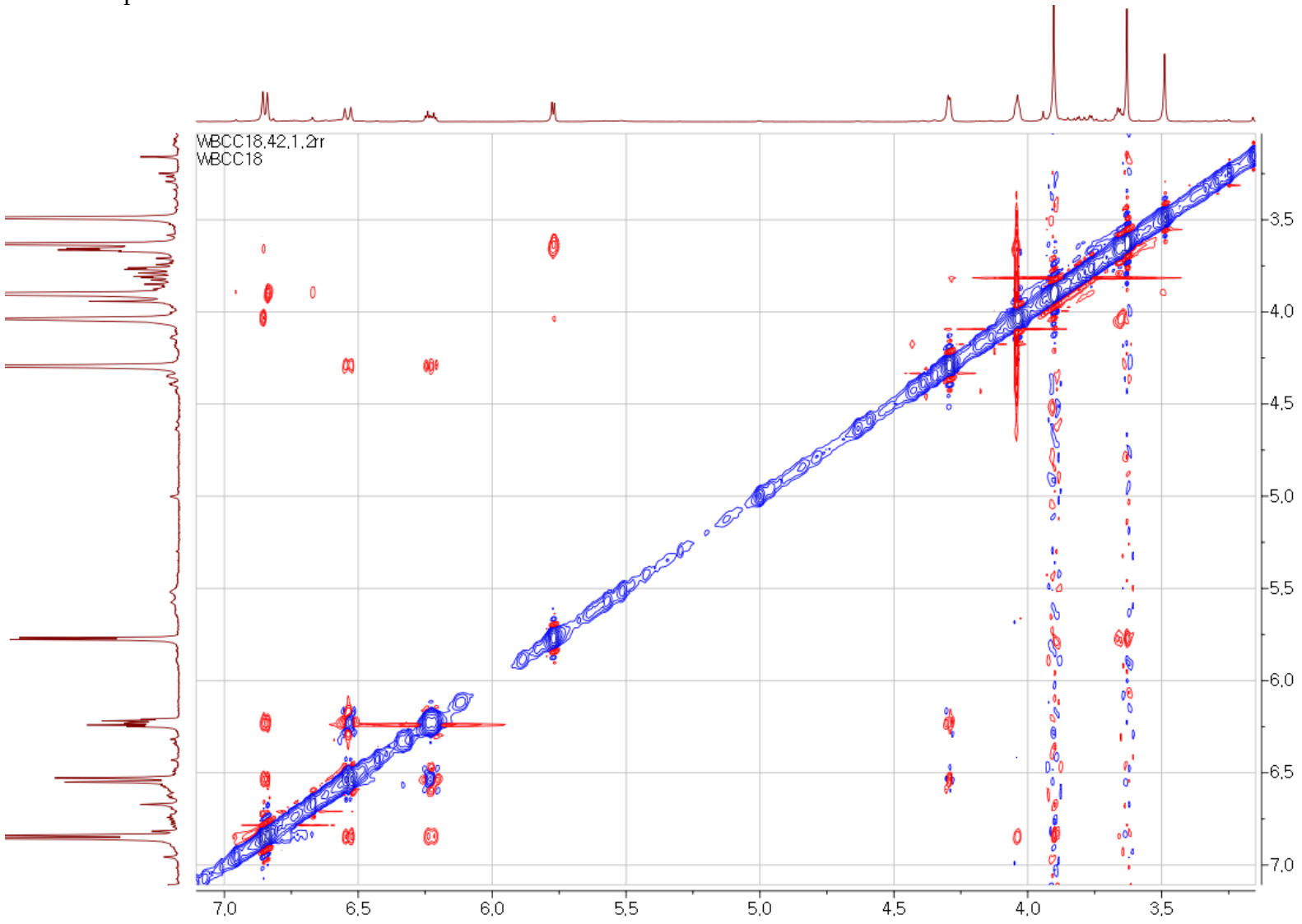
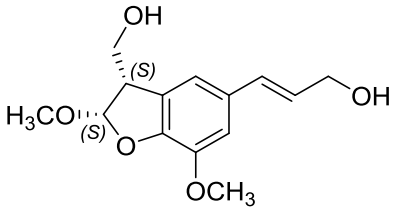
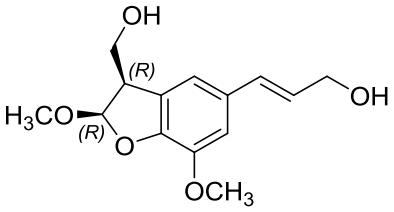


Figure S7. Two possible enantiomers of **1**.



1'*S*,2'*S*-**1**



1'*R*,2'*R*-**1**

Table S1. Boltzmann populations of conformers of **1**.

Conformer	E_{zpe}	U	H	G
1	23.1%	23.3%	23.3%	23.6%
2	24.0%	23.9%	23.9%	25.3%
3	18.8%	18.9%	18.9%	17.9%
4	19.2%	19.0%	19.0%	20.1%
5	5.0%	5.1%	5.1%	3.7%
6	3.7%	3.7%	3.7%	3.4%
7	3.0%	2.9%	2.9%	3.2%
8	3.2%	3.2%	3.2%	2.8%

Table S2. Computed thermodynamic data and zero-point vibrational energy of **1** (gas phase) used for chemical shift values [B3LYP/6-31+(d,p)]

Conformer	**E_{zpe}**	**U**	**H**	**G**
1	-920.141867	-920.12206	-920.121116	-920.191669
2	-920.141903	-920.122084	-920.12114	-920.191735
3	-920.141672	-920.121864	-920.12092	-920.19141
4	-920.141692	-920.121868	-920.120924	-920.191518
5	-920.140416	-920.120623	-920.119679	-920.189919
6	-920.140134	-920.120314	-920.11937	-920.189826
7	-920.139937	-920.120086	-920.119141	-920.189777
8	-920.139989	-920.120178	-920.119234	-920.189641

E_{zpe}, U, H, and G stand for zero-point energy, thermal energy, thermal enthalpy and Gibbs free energy, respectively.