

**Versispiroketal A, an unusual tetracyclic bridged spiroketal from the
sponge-associated fungus *Aspergillus versicolor* SCSIO 41013**

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TTGGAAGAGAAAAAGATGTAACAAGGTTTCCGTAGGTGAACCTGCGGAA
GGATCATTACTGAGTGCGGGCTGCCTTCGGGCGCCCAACCTCCCACCCGT
GACTACCTAACACTGTTGCTTCGGCGGGGAGCCCTCTCGGGGGCGCGCCG
CCGGGGACTACTGAACTTCATGCCTGAGAGTGATGCAGTCTGAGTCTGAA
TATAAAATCAGTCAAACTTTCAACAATGGATCTCTTGGTTCCGGCATCGA
TGAAGAACGCAGCGAACTGCGATAAGTAATGTGAATTGCAGAATTCAGTG
AATCATCGAGTCTTTGAACGCACATTGCGCCCCCTGGCATTCCGGGGGGC
ATGCCTGTCCGAGCGTCATTGCTGCCATCAAGCCCGGCTTGTGTGTTGGG
TCGTCGTCCCCCGGGGGACGGGCCCGAAAGGCAGCGGCAGCGGCACCGTGT
CCGGTCCTCGAGCGTATGGGGCTTTGTCACCCGCTCGATTTAGGGCCGGCC
GGGCGCCAGCCGACGTCCAACCATTTTTCTTCAGGTTGACCTCGGATCAG
GTAGGGATACCCGCTGAACTTAAGCATATCTAGACCGCGGAAGAAA

Figure S1. The ITS gene sequence data of *Aspergillus versicolor* SCSIO 41013

Table S1. Energies of 1 at MMFF94 force field.

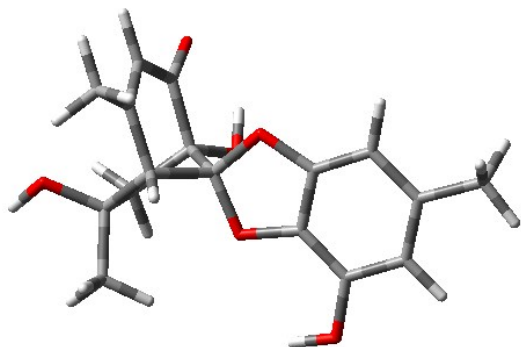
Configuration	Conformer	Energy (kcal/mol)	Population (%)
(1R,5S,6S,8R)-1	1	512.31	56.9
(1R,5S,6S,8R)-1	2	513.23	39.4
(1R,5S,6S,8R)-1	3	519.17	3.6
(1R,5S,6S,8R)-1	4	532.38	0.0

Table S2. Energies of 1 at B3LYP/6-31+g(d) level in methanol.

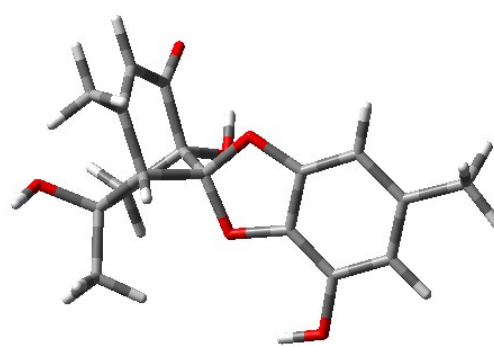
Configuration	Conformer	E (Hartree)	E (kcal/mol)	Population (%)
(1R,5S,6S,8R)-1	1	-1110.2925889	-696719.702460639	19.02
(1R,5S,6S,8R)-1	2	-1110.2930406	-696719.985906906	30.71
(1R,5S,6S,8R)-1	3	-1110.2930227	-696719.974674477	30.13

(1*R*,5*S*,6*S*,8*R*)-1 4 -1110.2926427 -696719.736220677 20.14

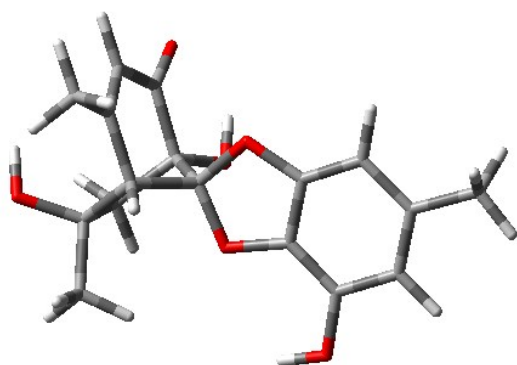
(1*R*,5*S*,6*S*,8*R*)-1



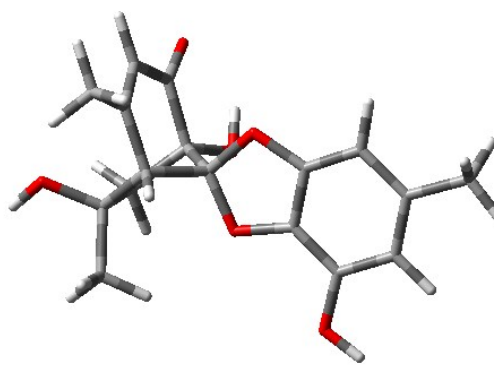
Conf.1 (19.02%)



Conf.2 (30.71%)



Conf.3 (30.13%)



Conf.4 (20.14%)

Figure S2. The optimized conformers and equilibrium populations of **1**

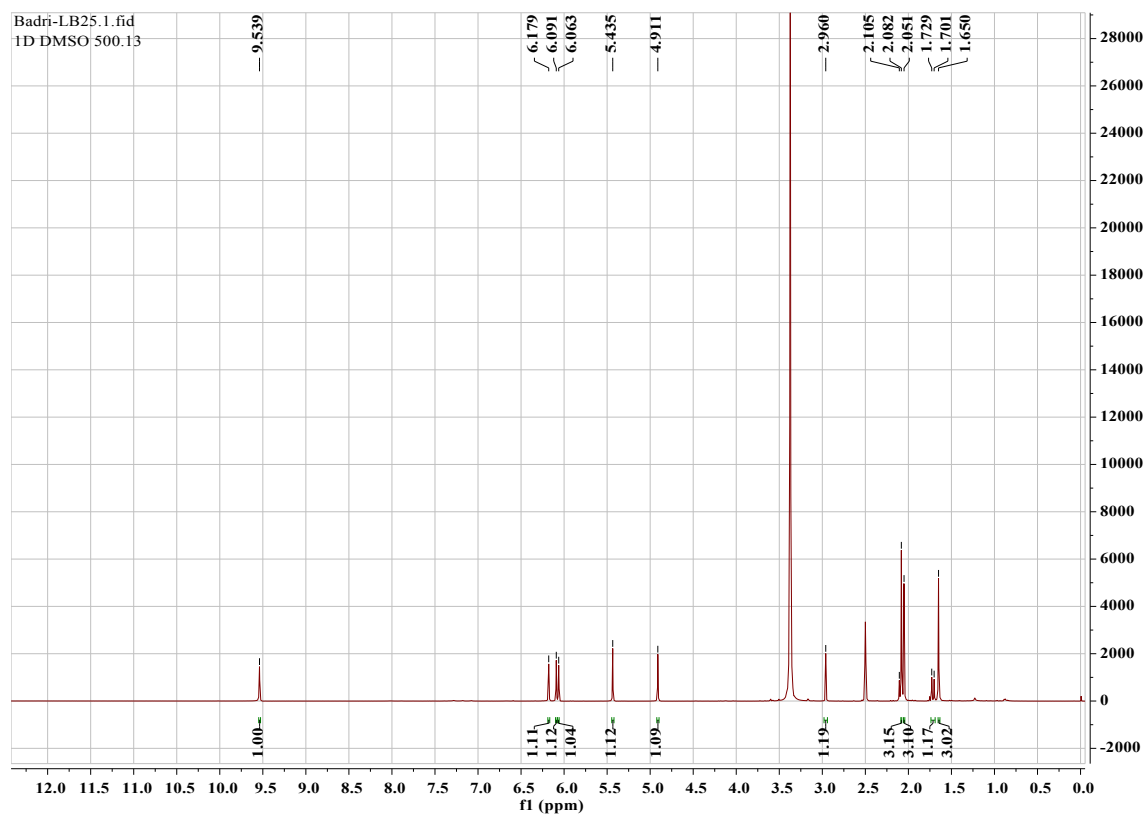
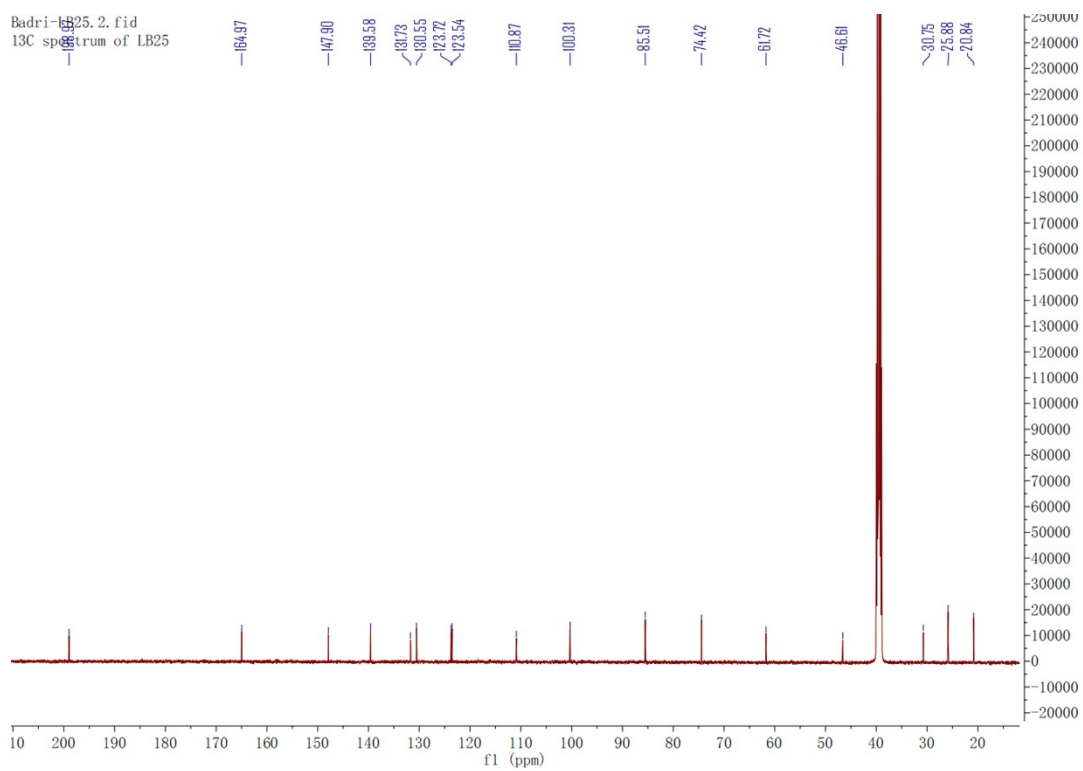


Figure S3. ^1H NMR spectrum of versispiroketal A (**1**) ($\text{DMSO-}d_6$, 500 MHz)



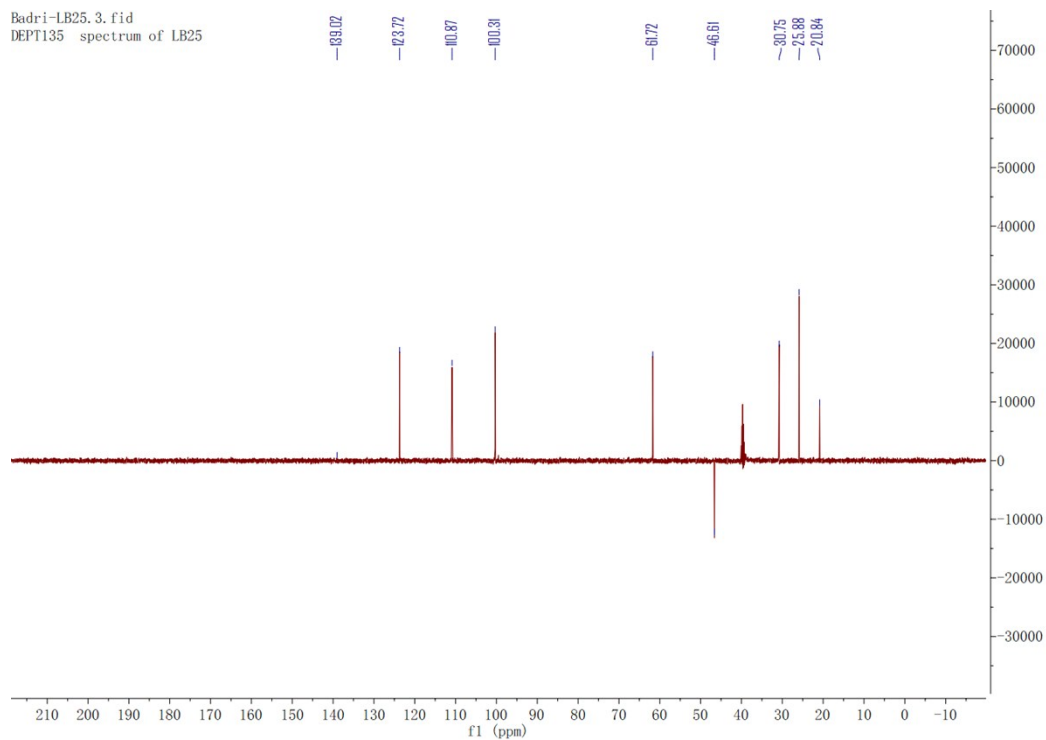


Figure S4.

^{13}C NMR and DEPT spectra of versispiroketal A (**1**) (DMSO- d_6 , 125 MHz)

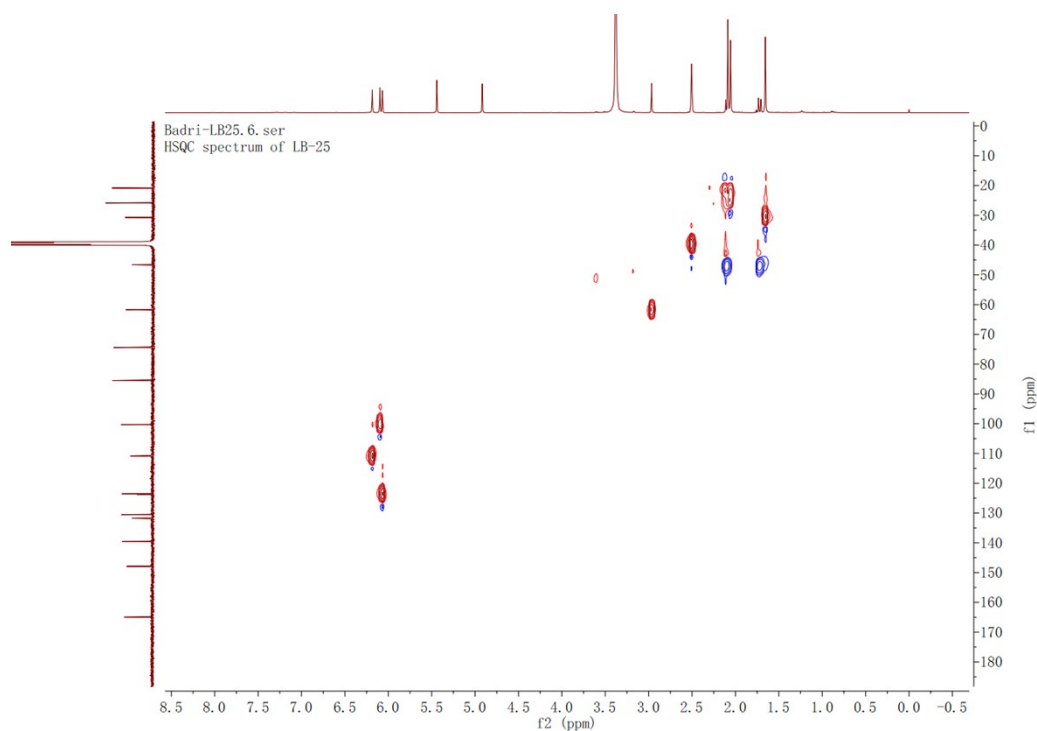


Figure S5. HSQC spectrum of versispiroketal A (**1**) (DMSO- d_6)

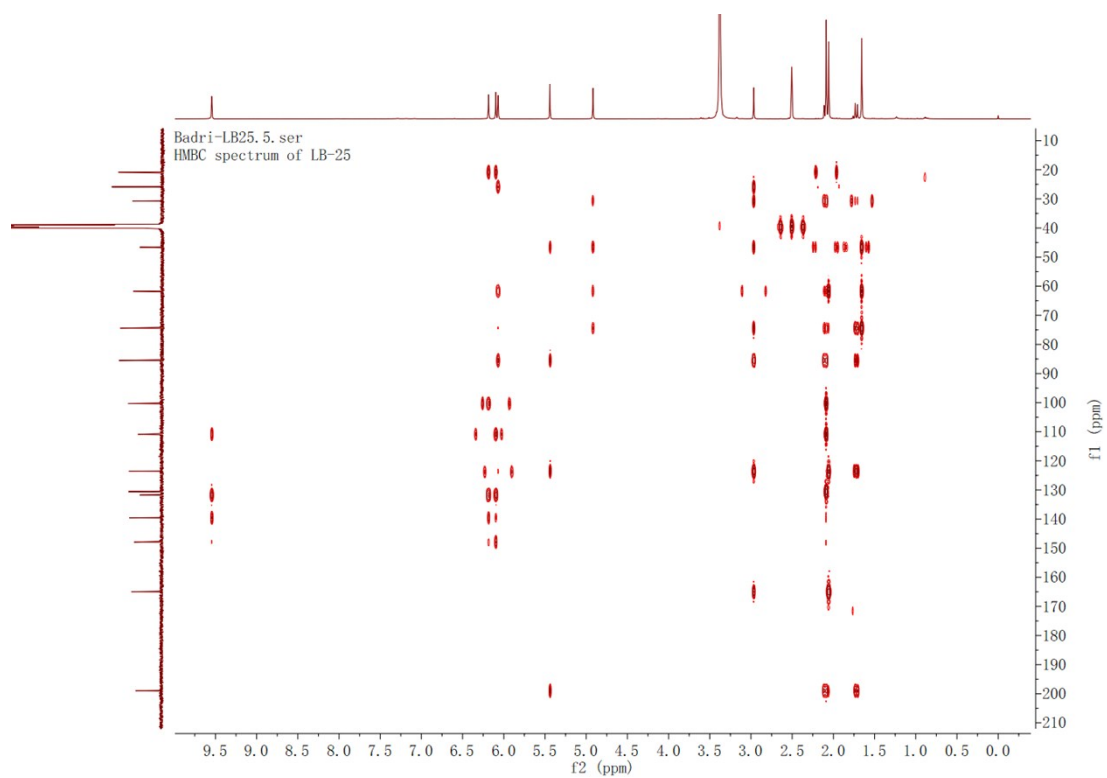


Figure S6. HMBC spectrum of versispiroketal A (**1**) (DMSO- d_6)

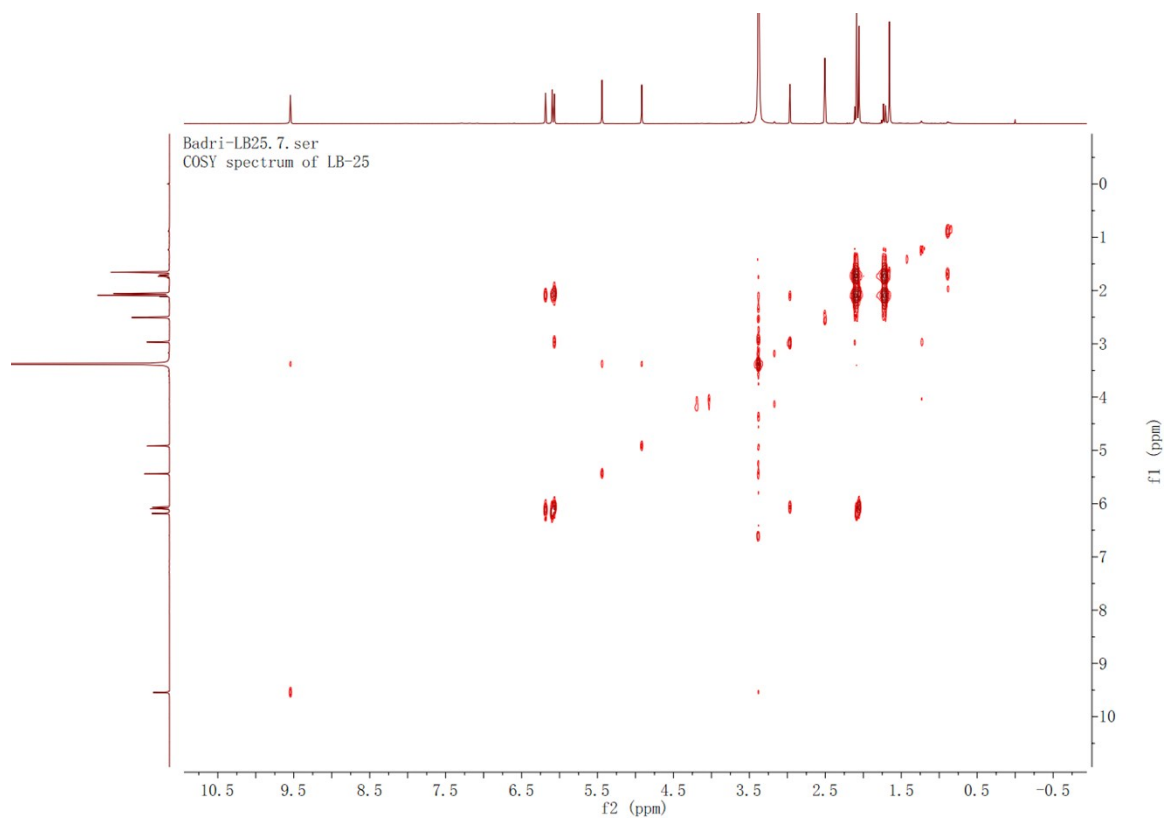


Figure S7. ^1H - ^1H COSY spectrum of versispiroketal A (**1**) (DMSO- d_6)

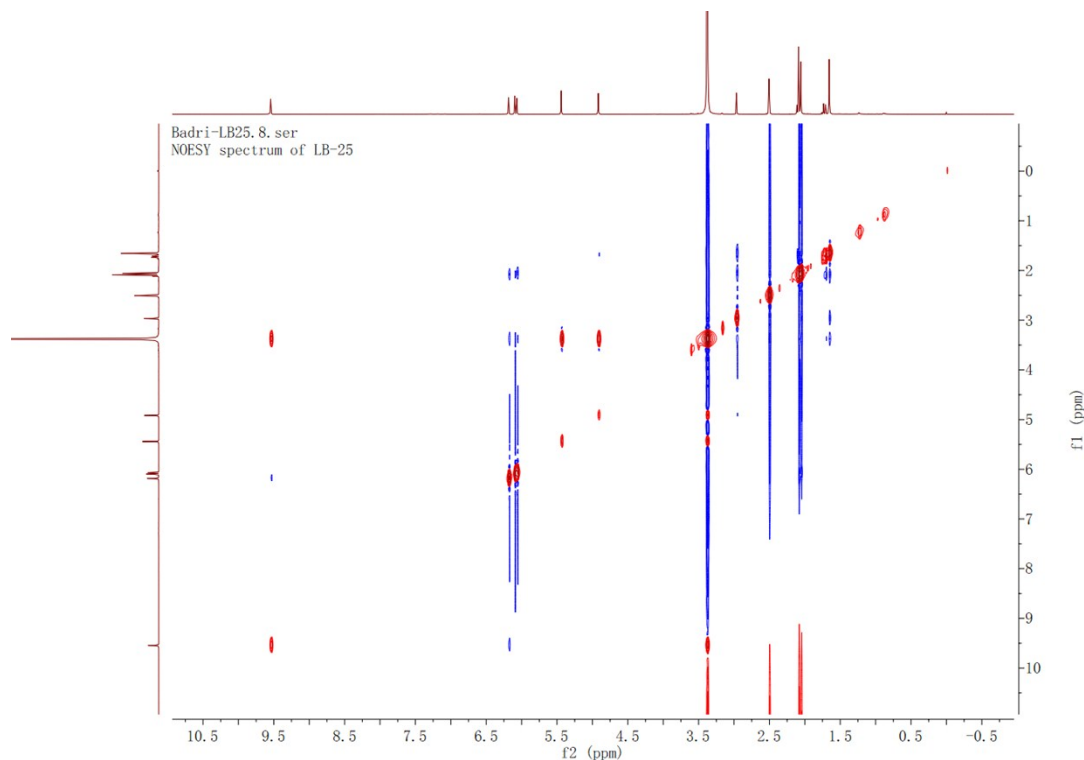
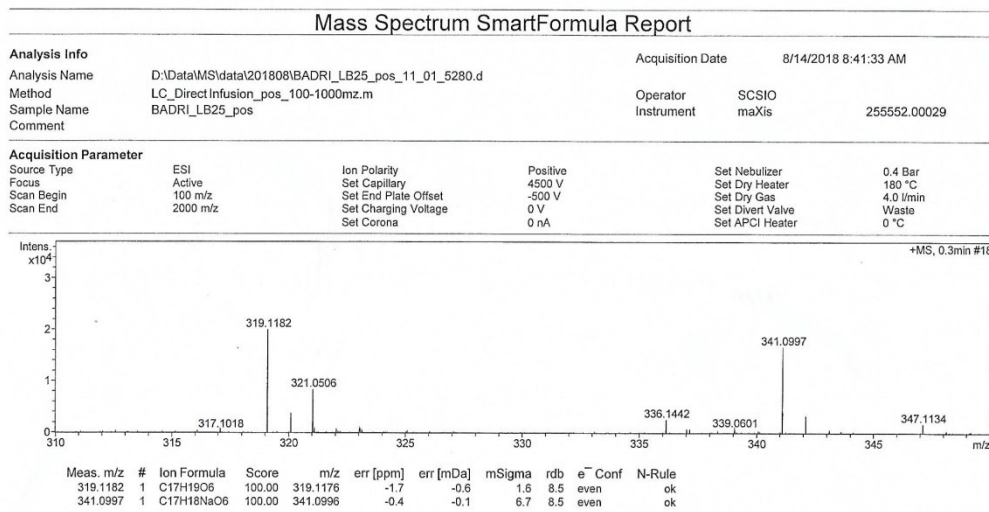


Figure S8. NOESY spectrum of versispiroketal A (1) (DMSO- d_6)



BADRI_LB25_pos_11_01_5280.d
Bruker Compass DataAnalysis 4.1

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Figure S9. HR-ESIMS spectrum of versispiroketal A (1)

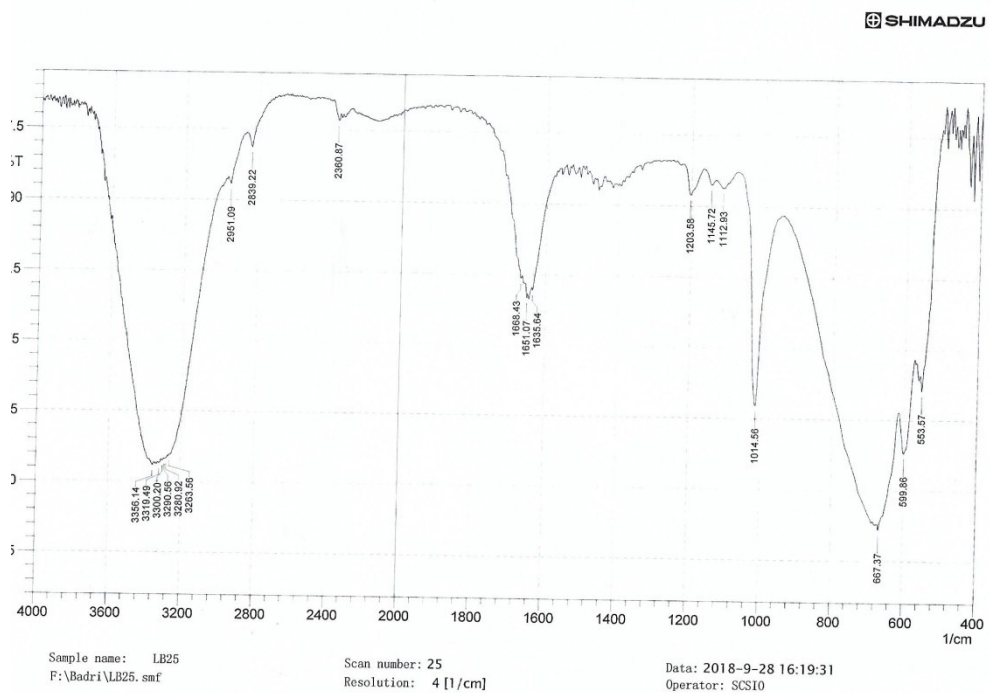


Figure S10. IR spectrum of versispiroketal A (1)

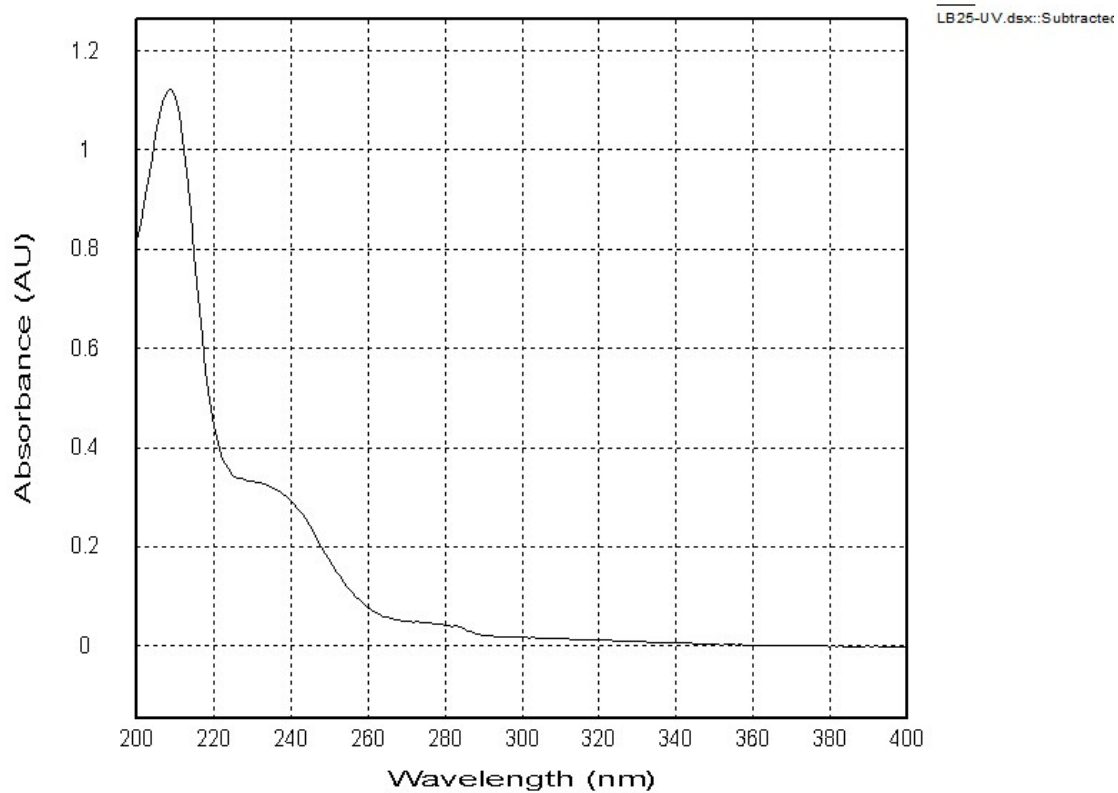


Figure S11. UV spectrum of versispiroketal A (1)