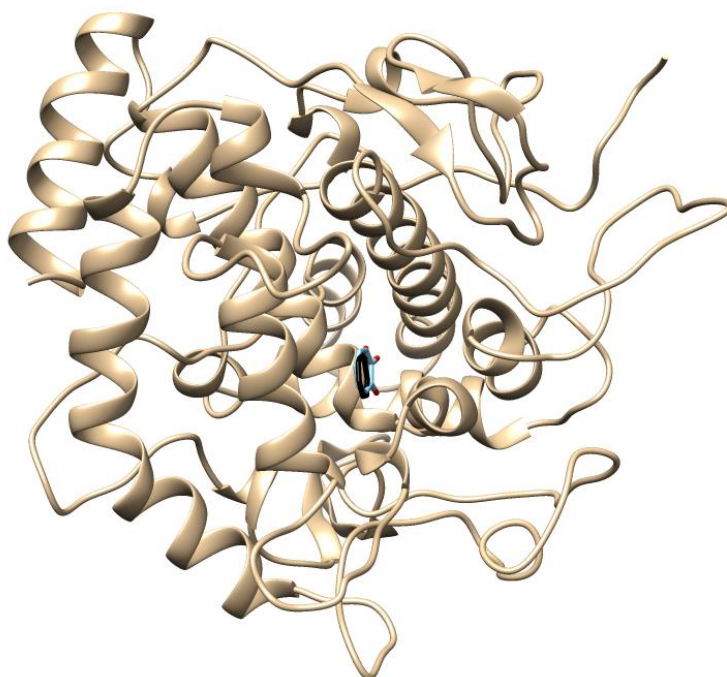


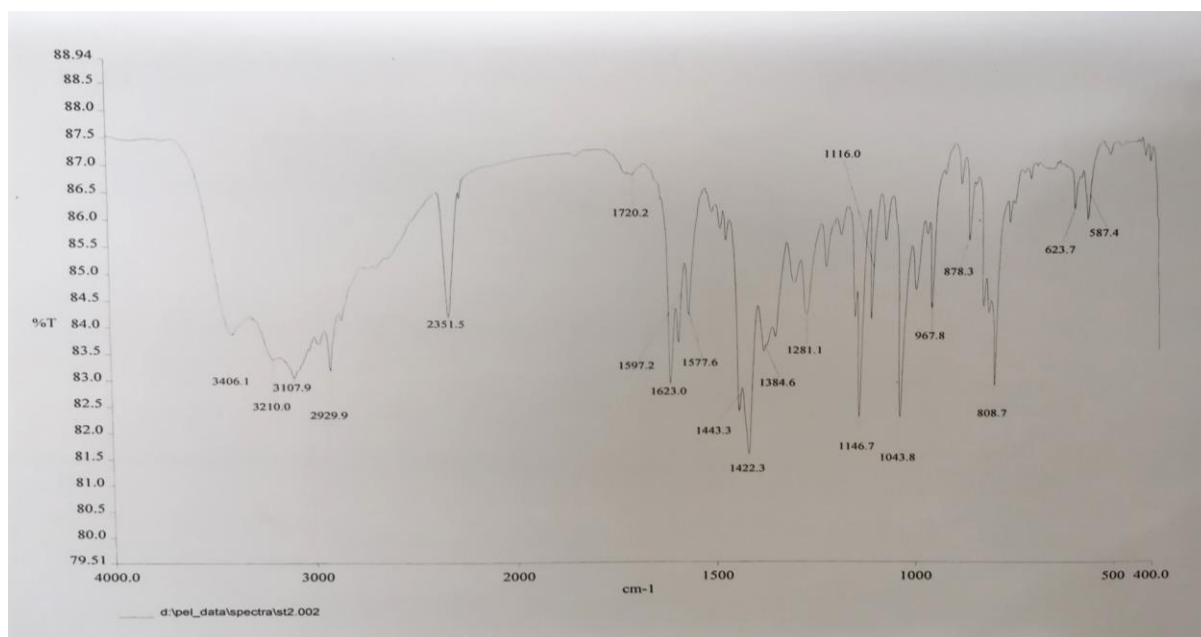
### Supplementary Materials

**Table S1.** A list of isolated compounds obtained from *S. taxoides*, downloaded from the PubChem database.

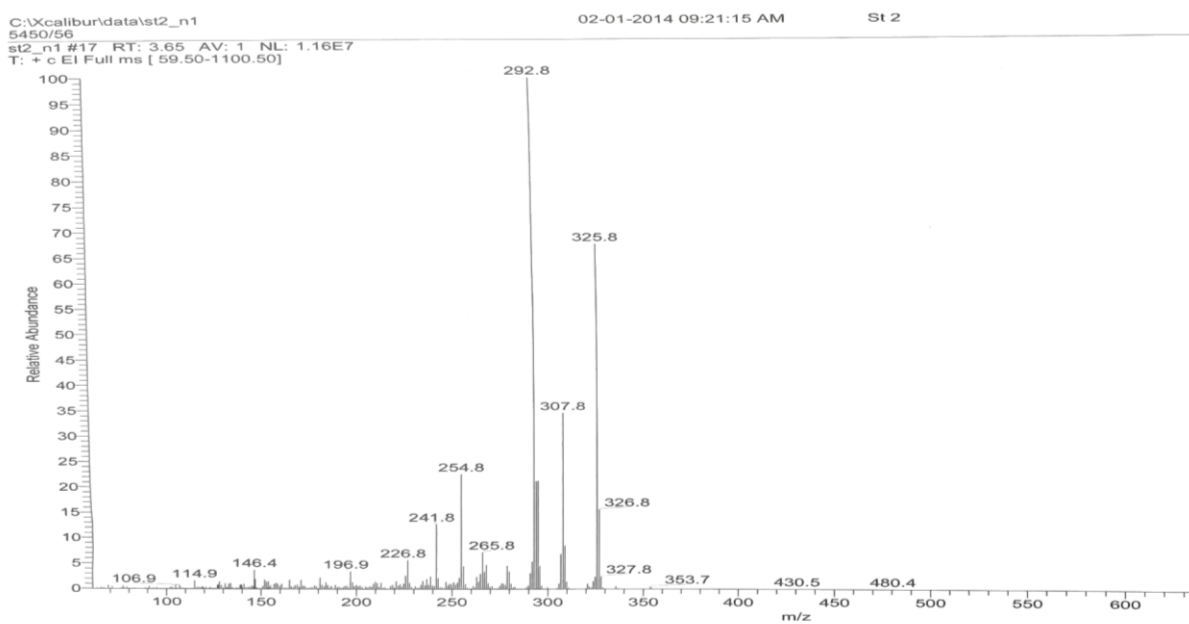
No.	Ligand	PubChem CID	Remark
1	Omega-Hydroxymoracin C	-	self-made from Moracin C
2	Moracin M	185848	-
3	Moracin C	155248	-
4	3,3',4,5'-Tetrahydroxybibenzyl	152444	-
5	piceatannol	667639	-



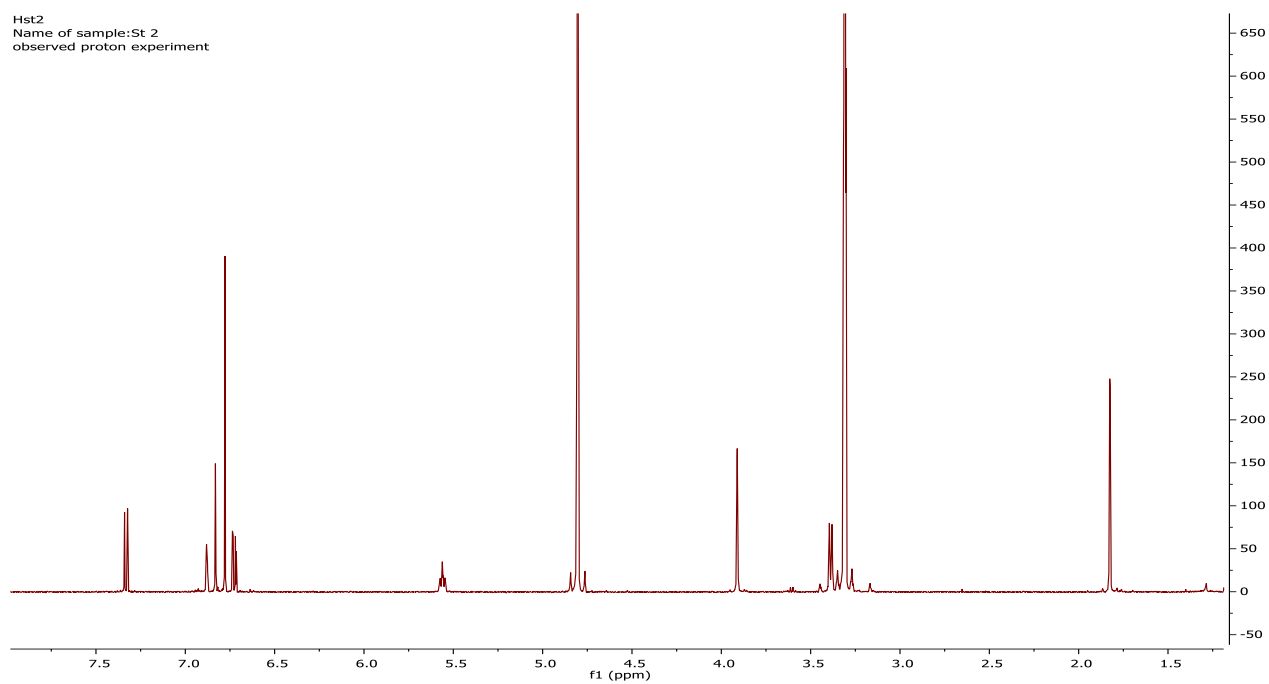
**Figure S1.** Docking protocol validation. Native tropolone structure (black color) locates in its original position. Re-docked tropolone (blue color) into its original pose overlays over native tropolone structure. The RMSD value of the re-docked tropolone is 1.038 Å.



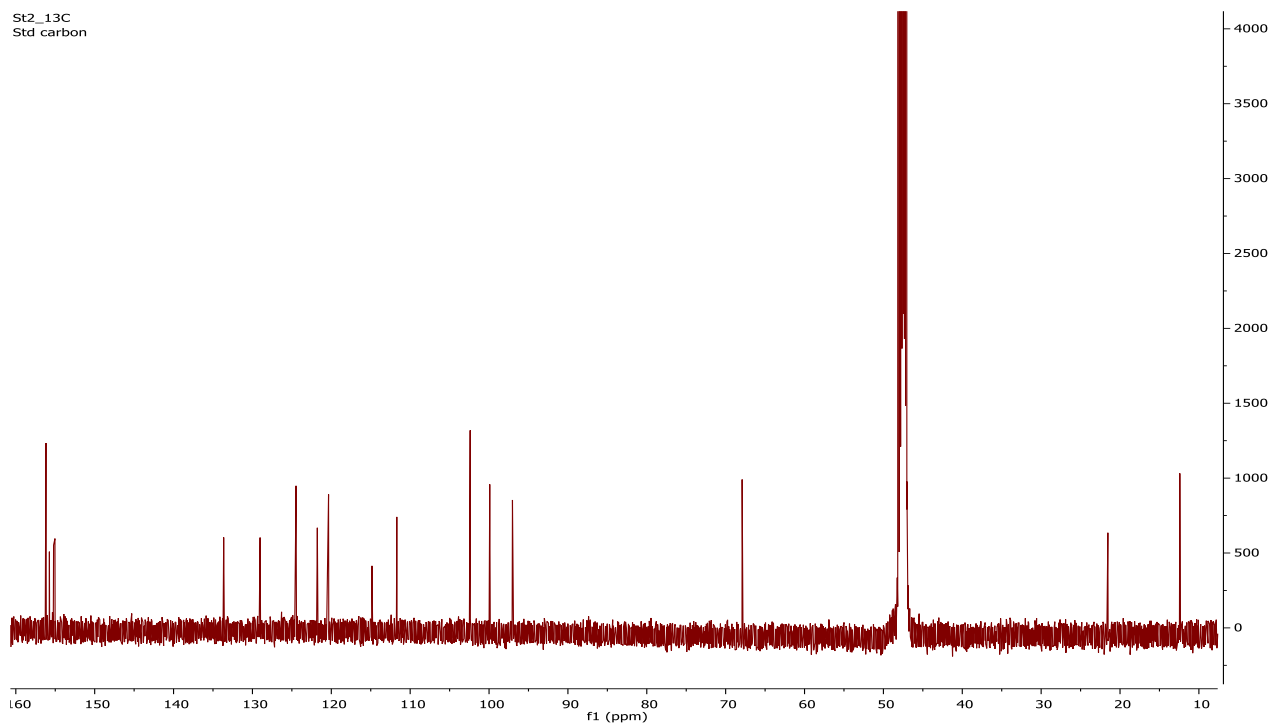
**Figure S2.** IR spectrum of  $\omega$ -hydroxymoracin C (KBr disc)



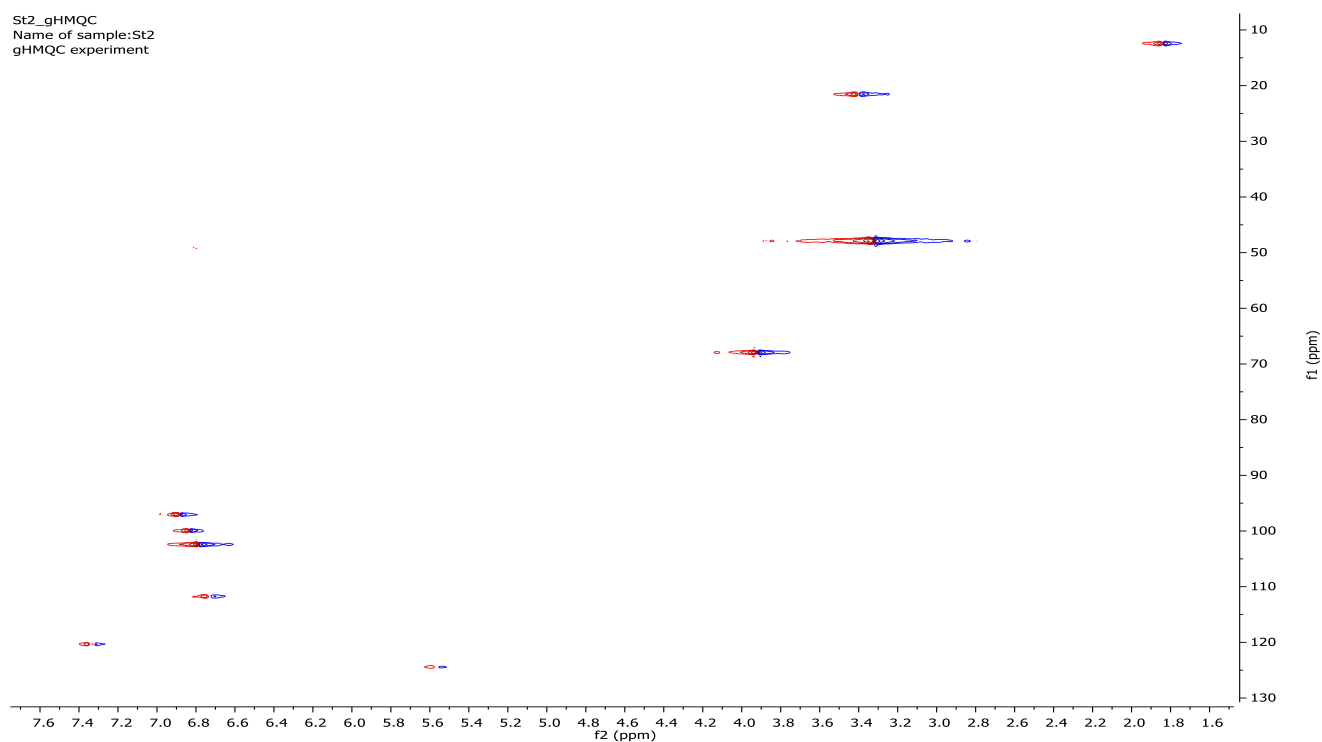
**Figure S3.** EI mass spectrum of  $\omega$ -hydroxymoracin C



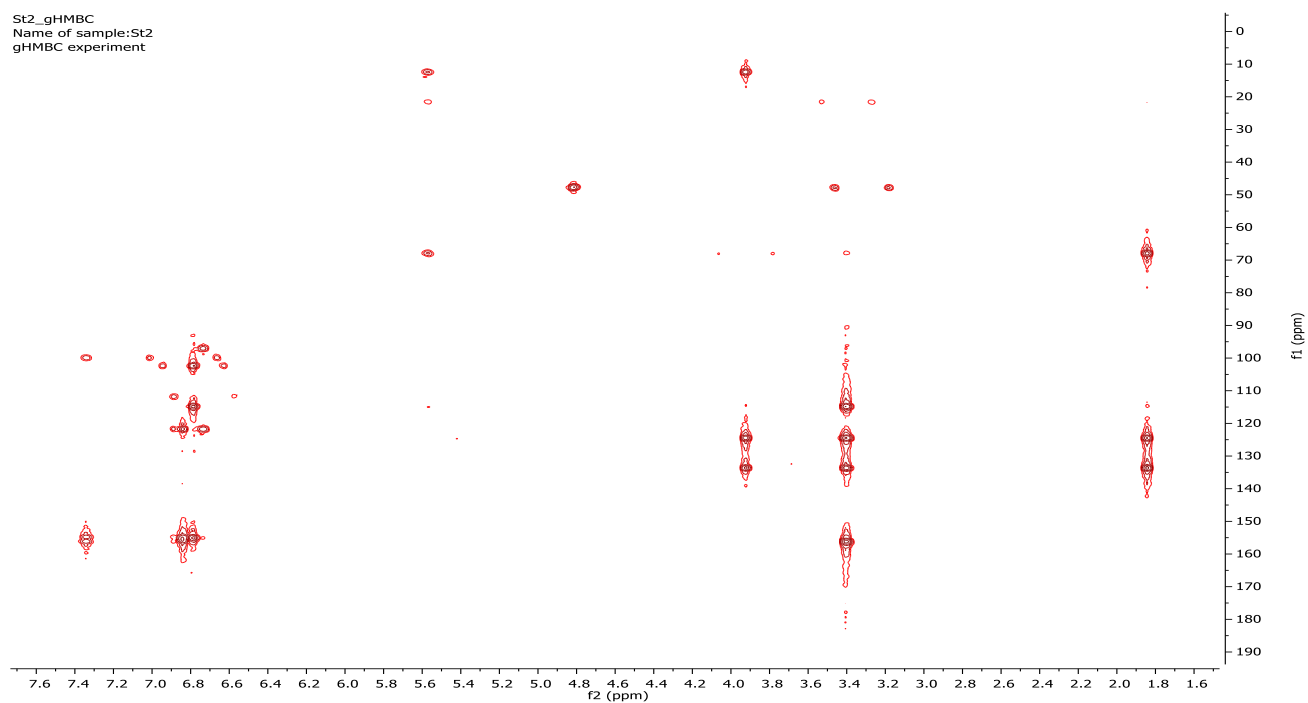
**Figure S4.** <sup>1</sup>H NMR spectrum of  $\omega$ -hydroxymoracin C



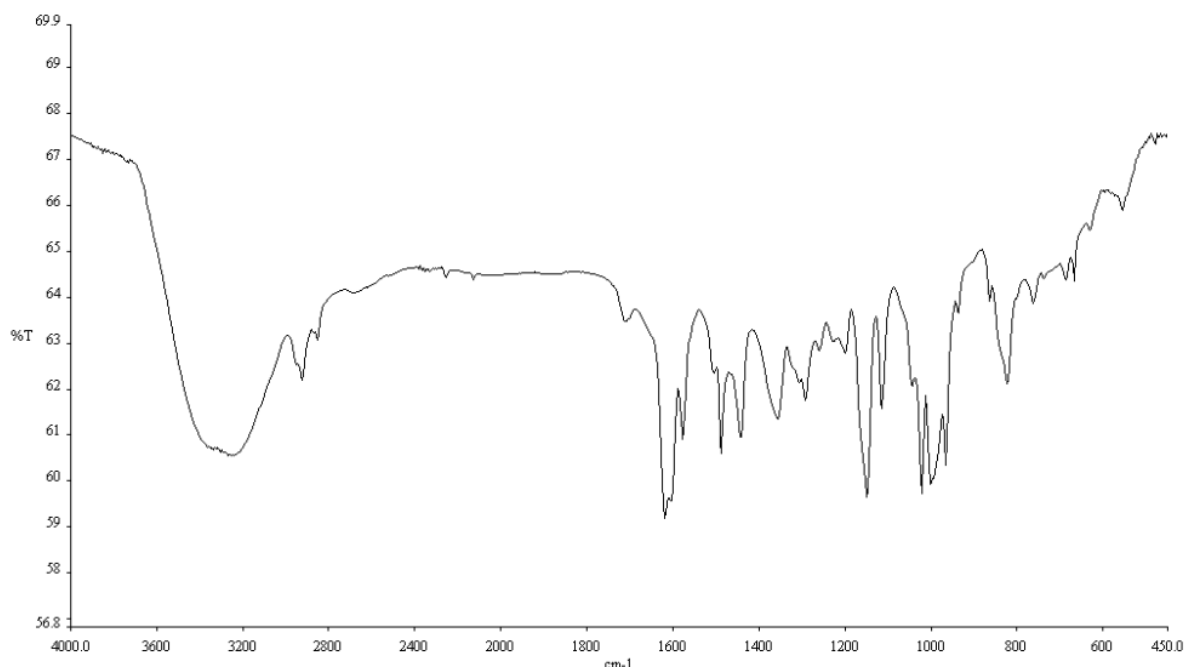
**Figure S5.** <sup>13</sup>C NMR spectrum of  $\omega$ -hydroxymoracin C



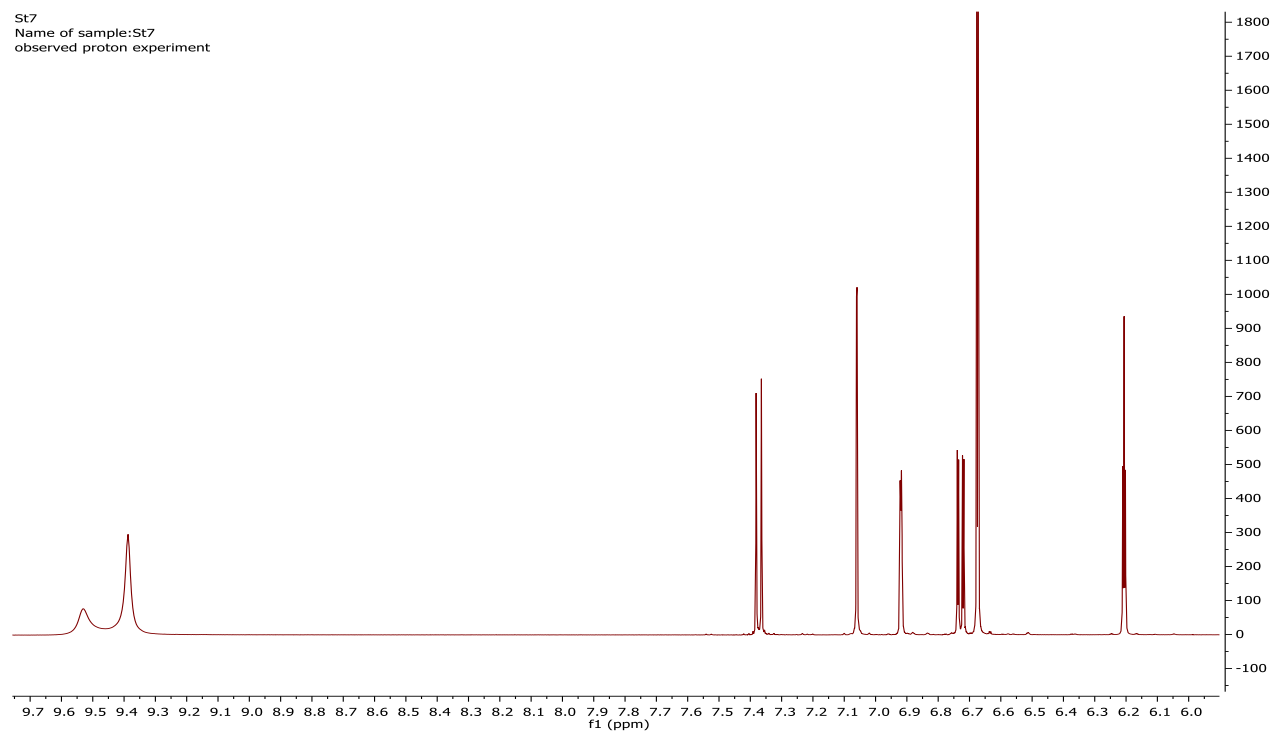
**Figure S6.** HMQC spectrum of  $\omega$ -hydroxymoracin C



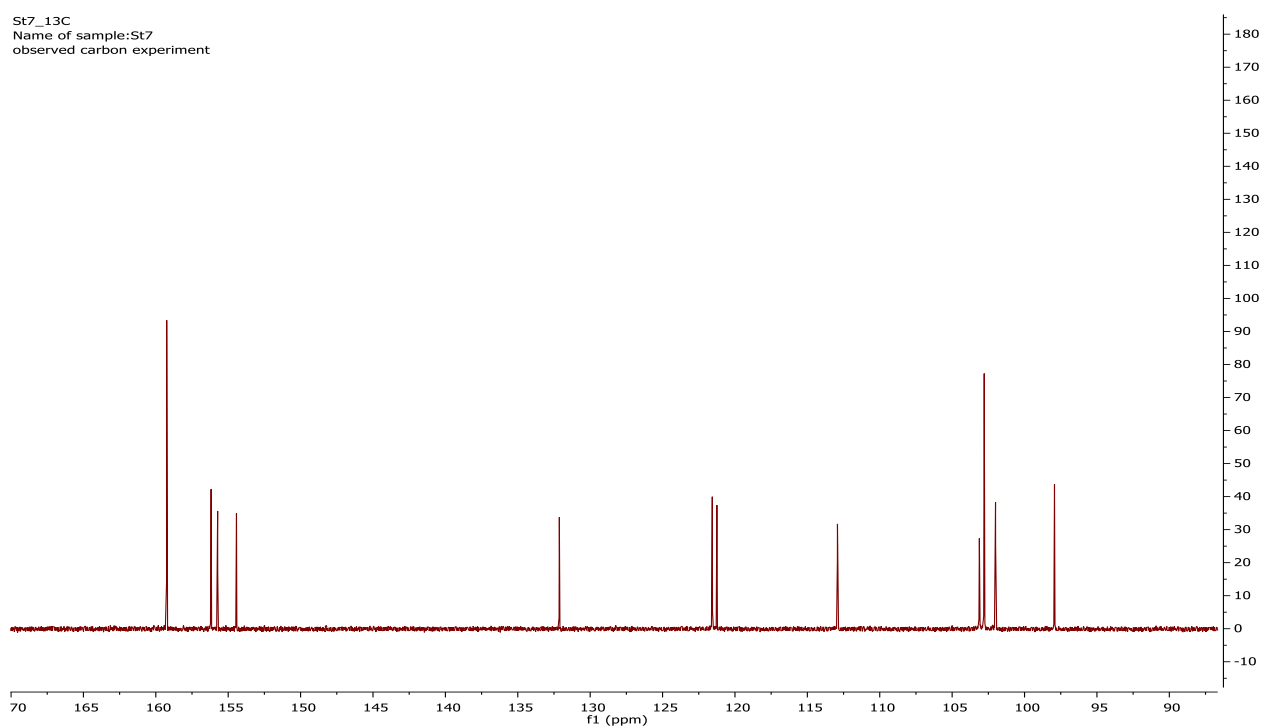
**Figure S7.** HMBC spectrum of  $\omega$ -hydroxymoracin C



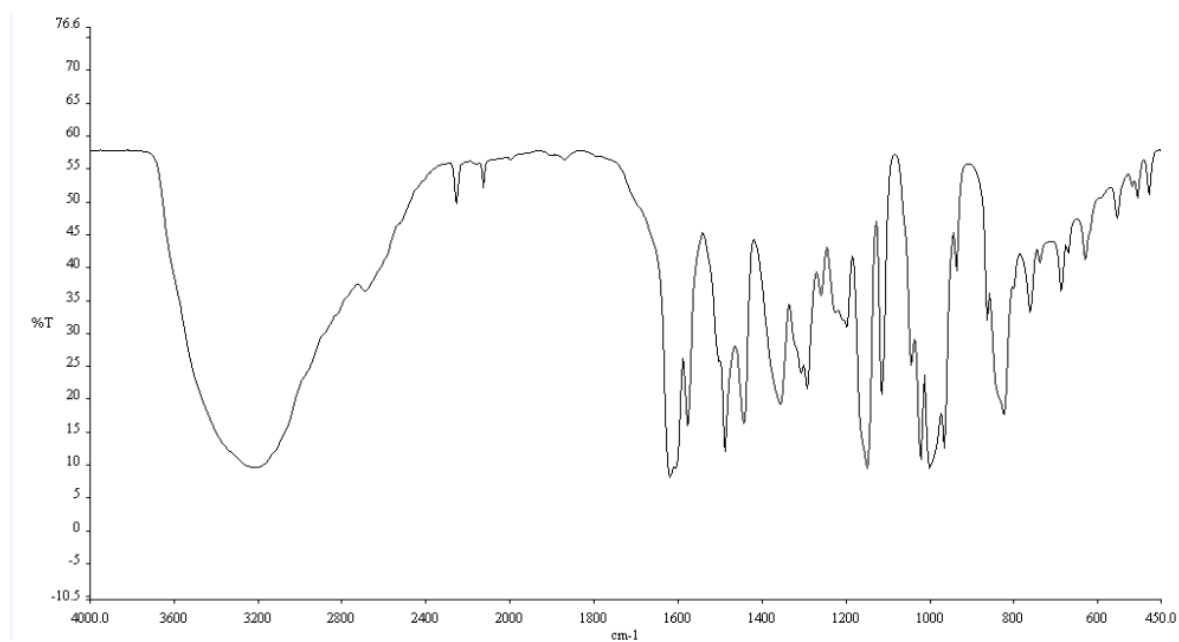
**Figure S8.** IR spectrum of moracin M (KBr disc)



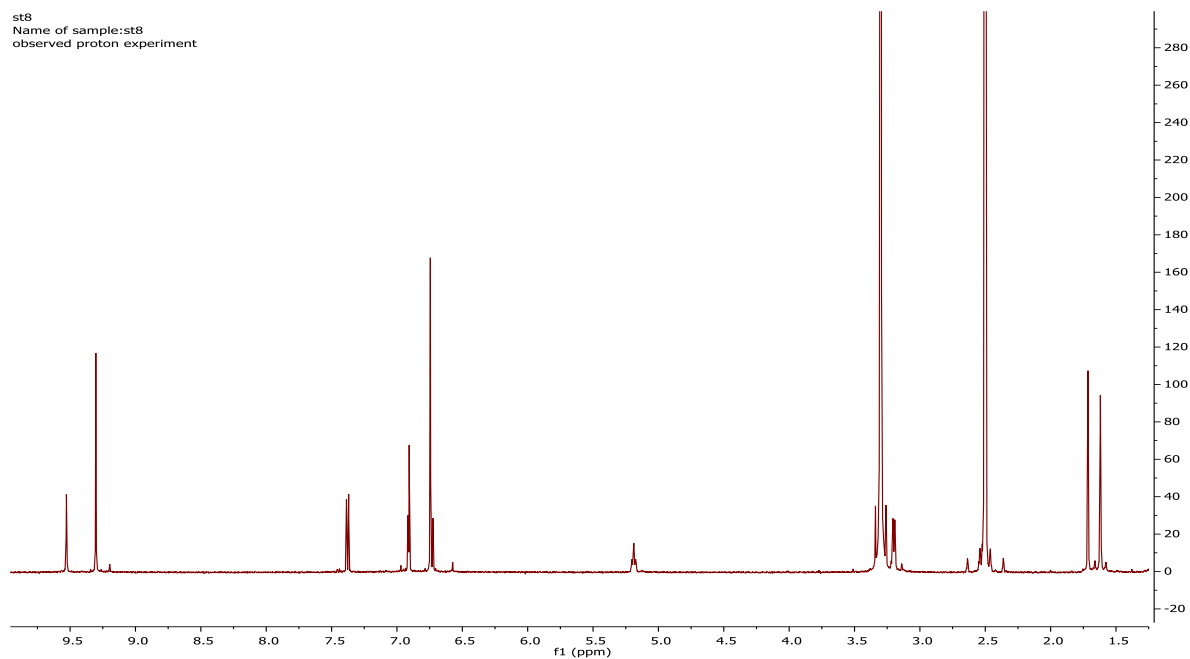
**Figure S9.**  $^1\text{H}$  NMR spectrum of moracin M



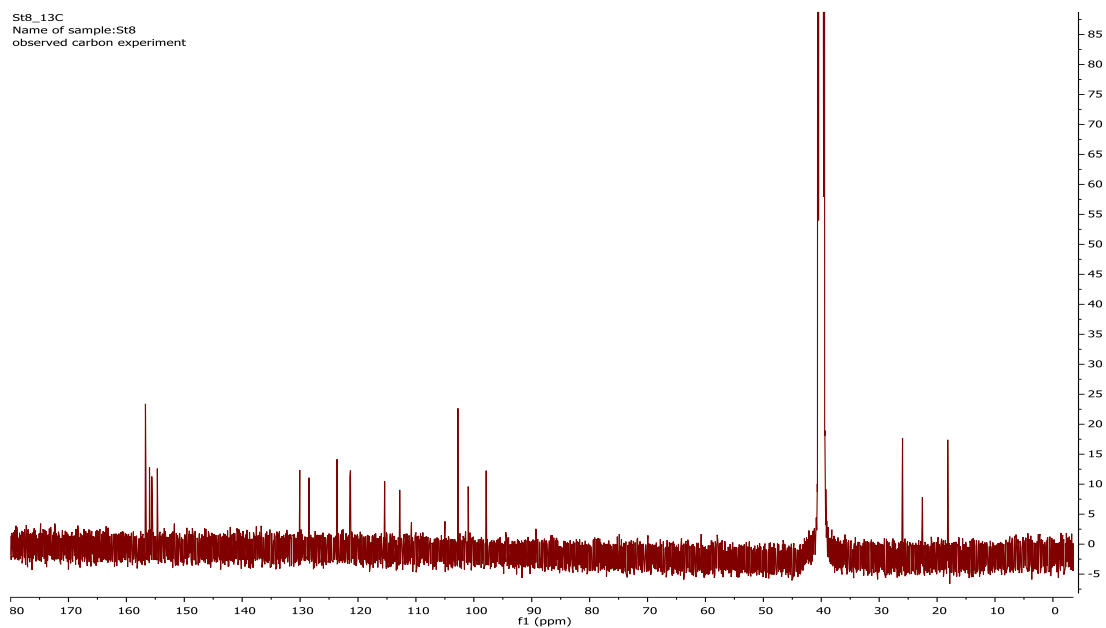
**Figure S10.**  $^{13}\text{C}$  NMR spectrum of moracin M



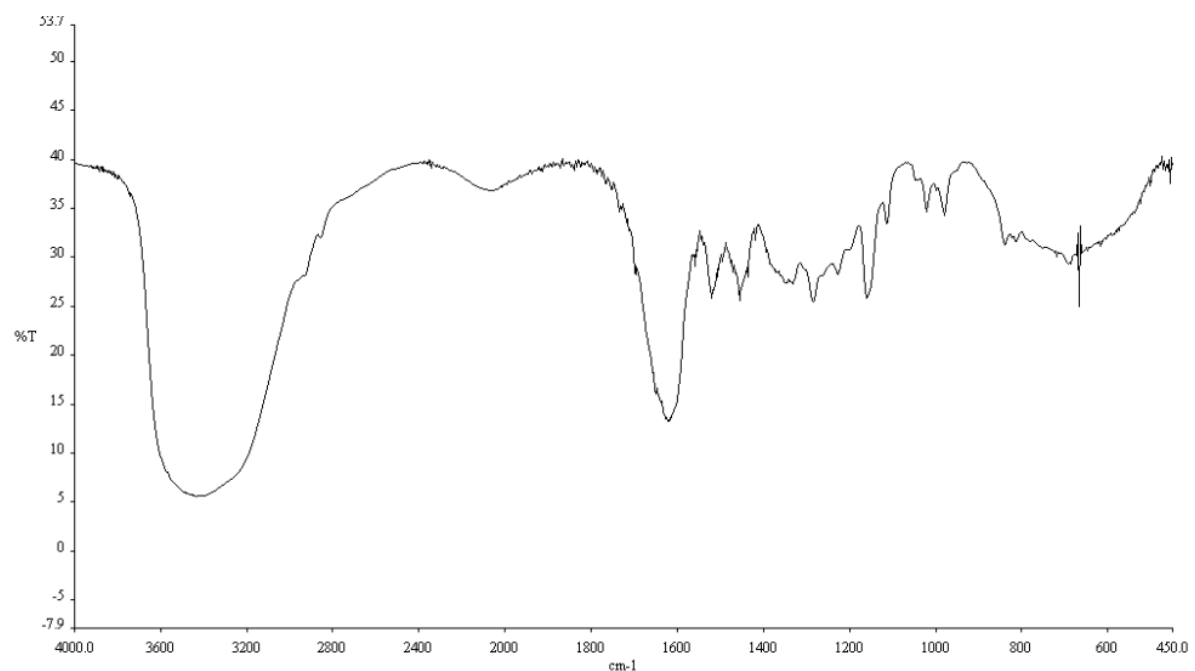
**Figure S11.** IR spectrum of moracin C (KBr disc)



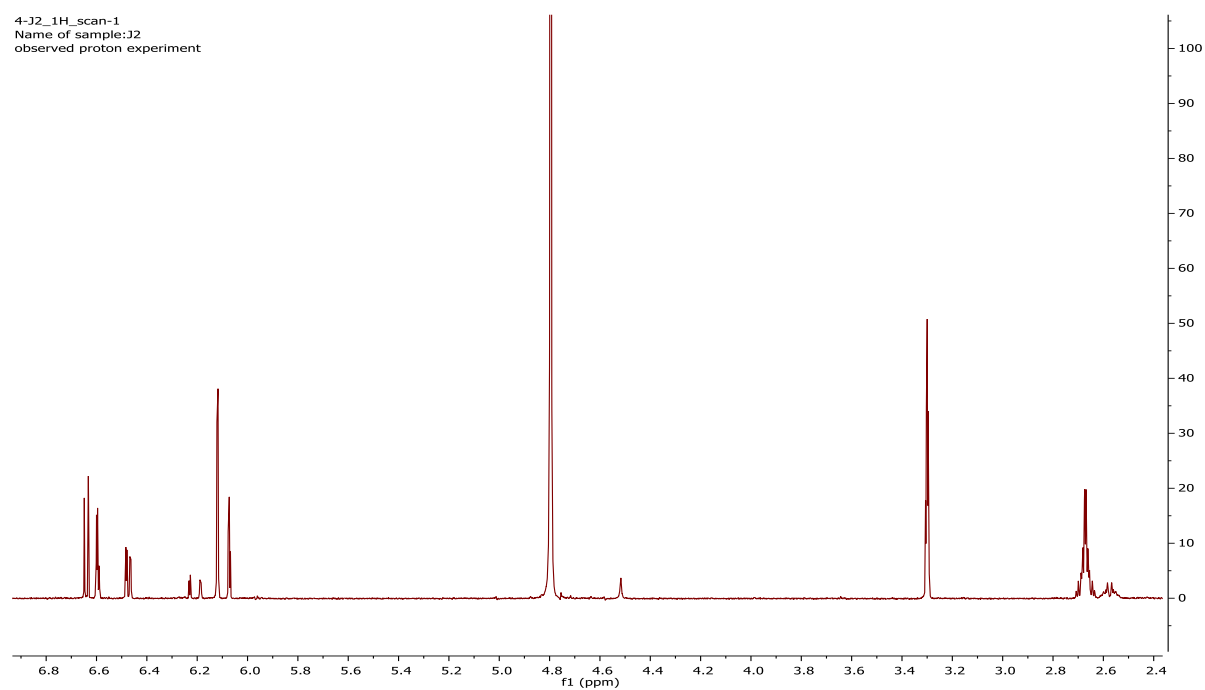
**Figure S12.**  $^1\text{H}$  NMR spectrum of moracin C



**Figure S13.**  $^{13}\text{C}$  NMR spectrum of moracin C

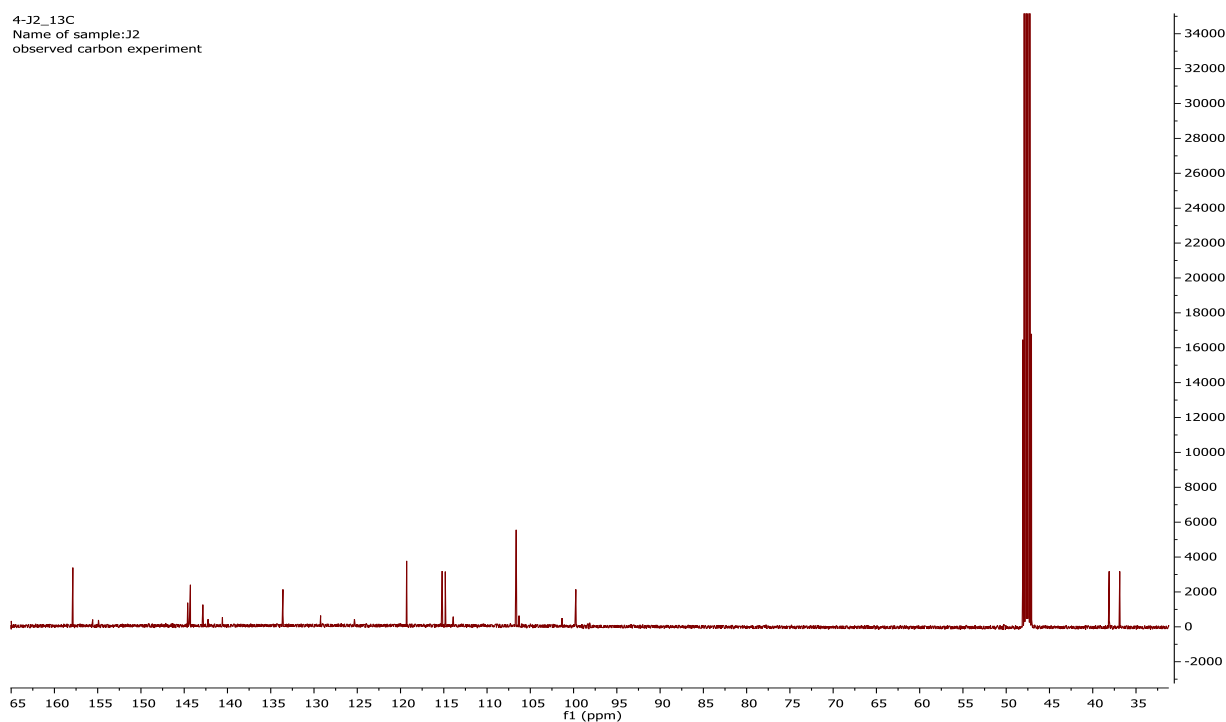


**Figure S14.** IR spectrum of 3, 4, 3', 5'-tetrahydroxybibenzyl (KBr disc)

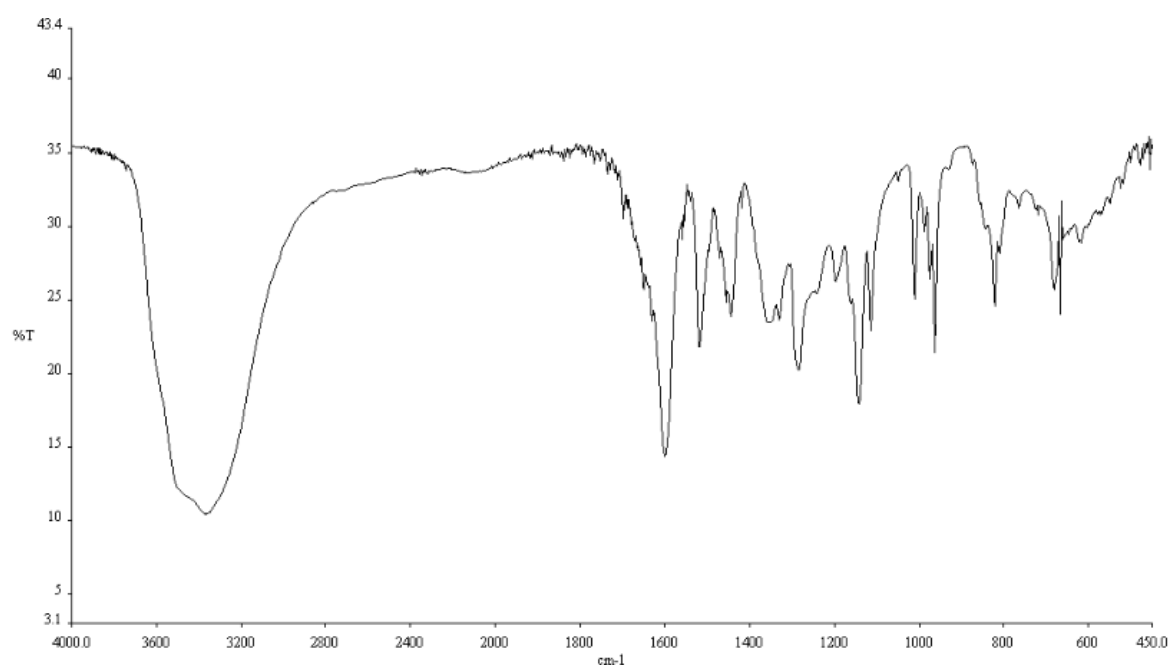


**Figure S15.** <sup>1</sup>H NMR spectrum of 3, 4, 3', 5'-tetrahydroxybibenzyl



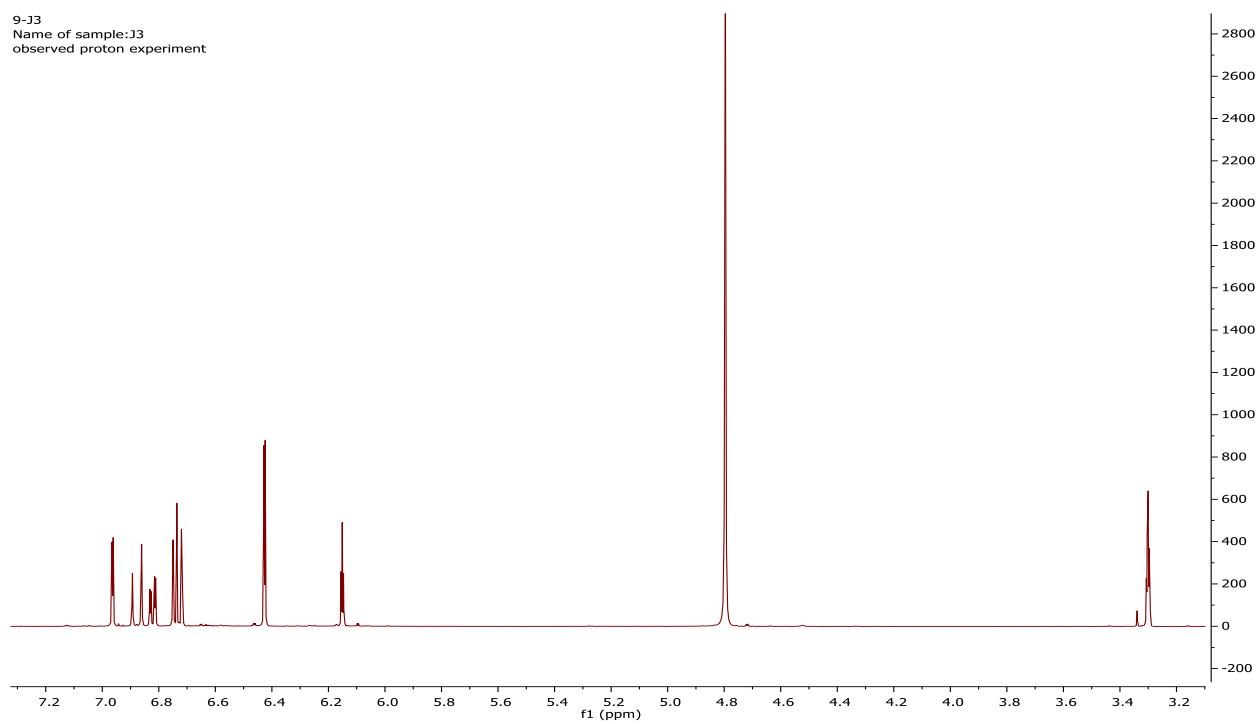


**Figure S16.**  $^{13}\text{C}$  NMR spectrum of 3, 4, 3', 5'-tetrahydroxybibenzyl



**Figure S17.** IR spectrum of piceatanol (KBr disc)

9-J3  
Name of sample:J3  
observed proton experiment



**Figure S18.**  $^1\text{H}$  NMR spectrum of piceatanol