Supporting information

Targeted isolation of cytotoxic sesquiterpene lactones from *Eupatorium fortunei* by the NMR annotation tool, SMART 2.0

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Figure S1. Extracts and sub-fractions of cytotoxic activity against five cell lines

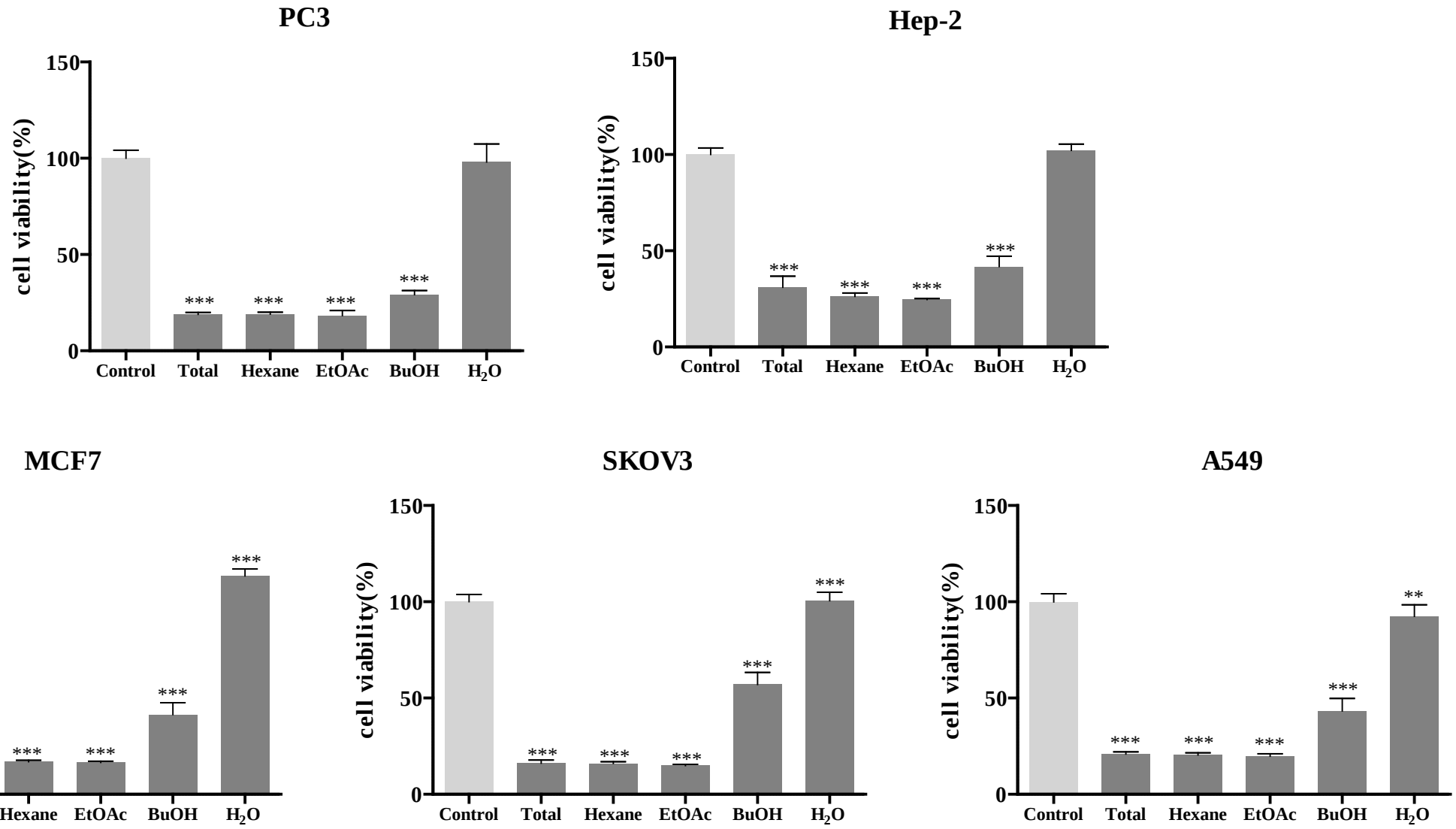
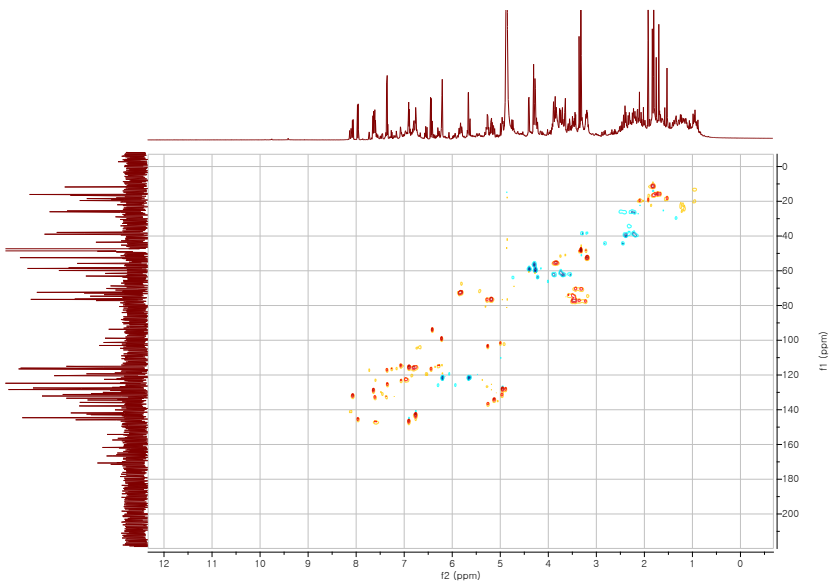
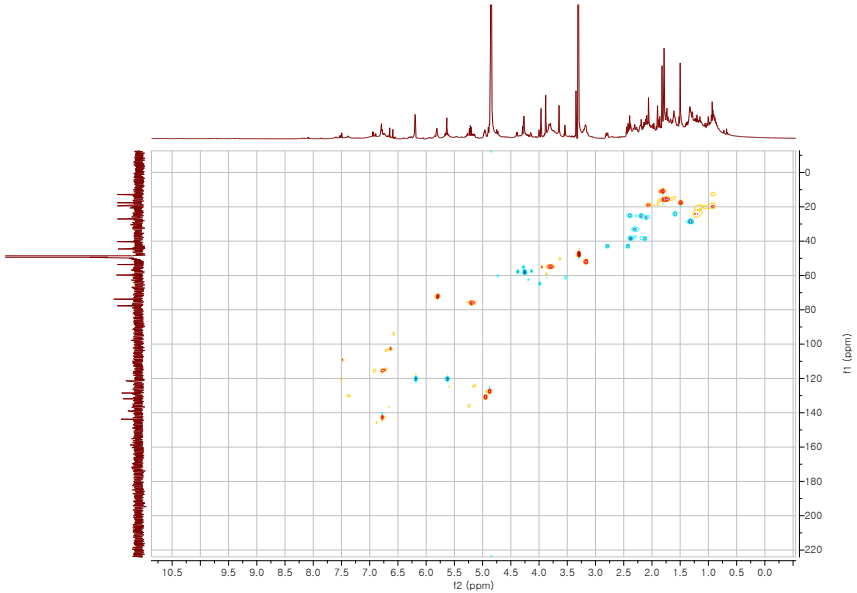


Figure S2. The HSQC spectrum of E2 and E3

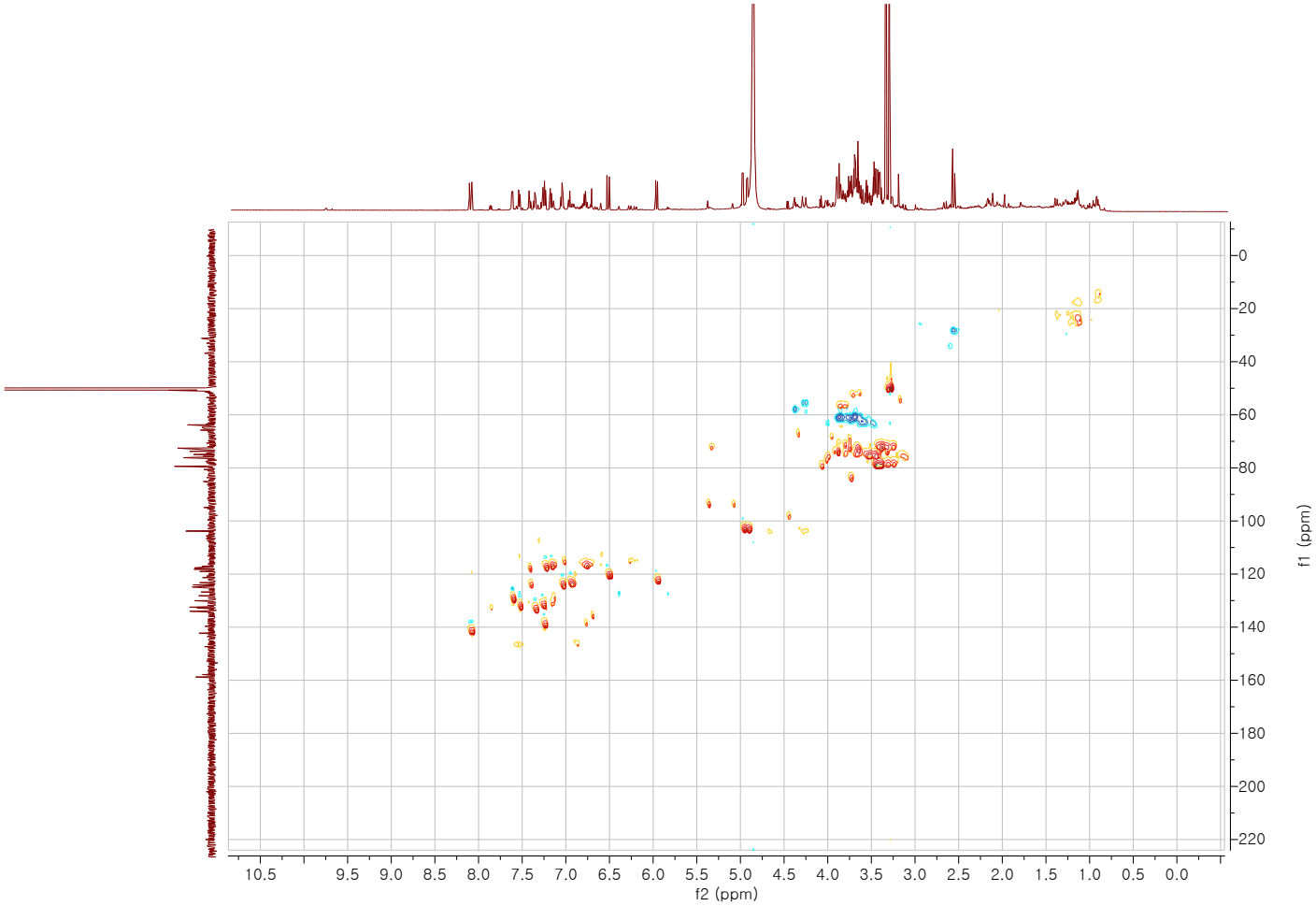


E2



E3

Figure S3. The HSQC spectrum and sunburst plot of E1



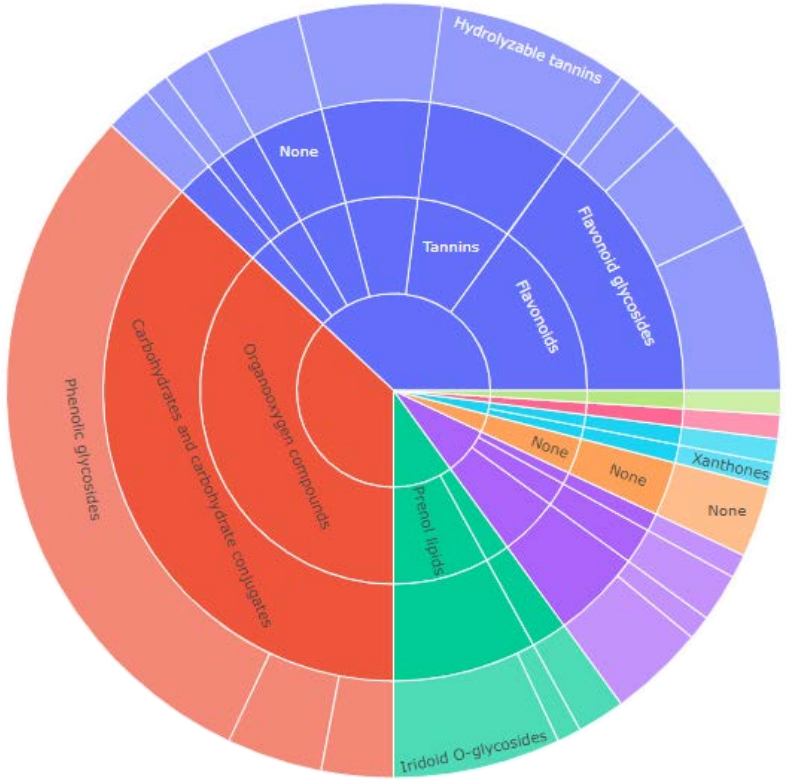
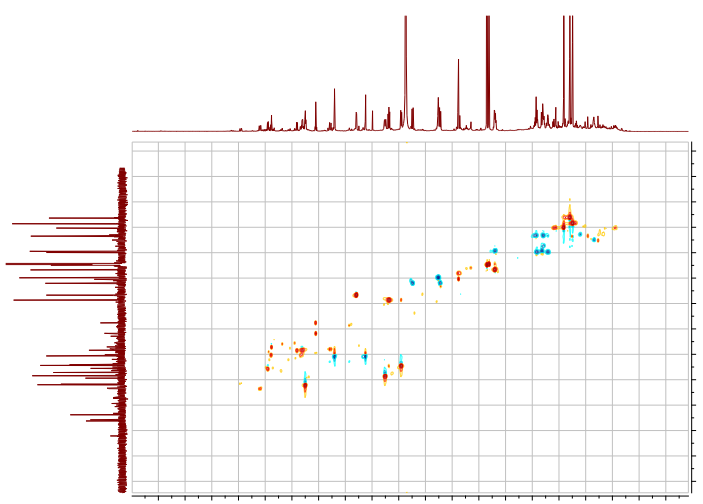
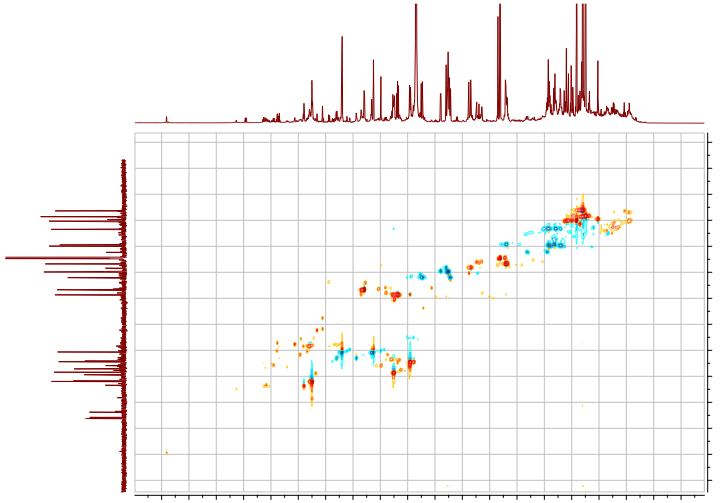


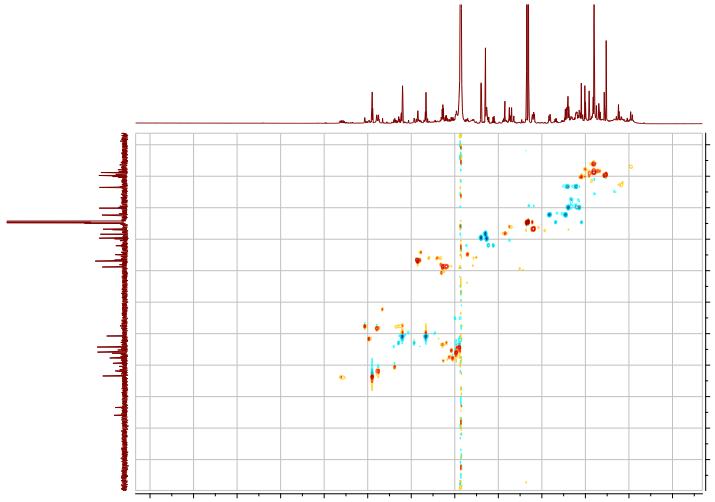
Figure S4. The HSQC spectrum of E2-4 , E2-5, E2-6 and E2-7



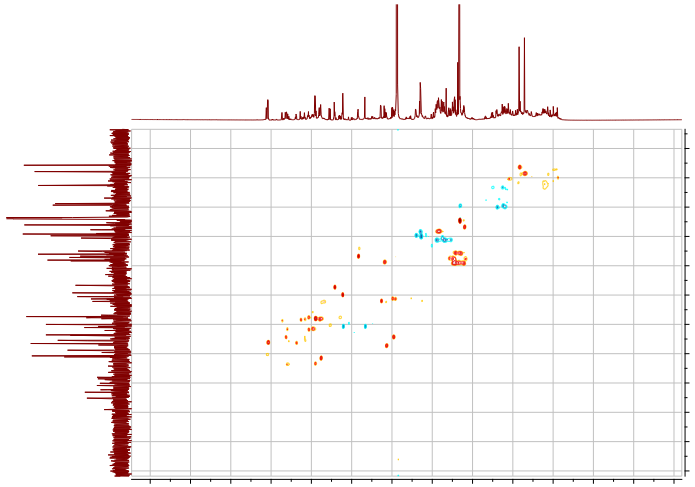
E2-4



E2-5



E2-6



E2-7

Figure S5. The structures of compounds predicted for sub-fraction E2-4 using SMART 2.0

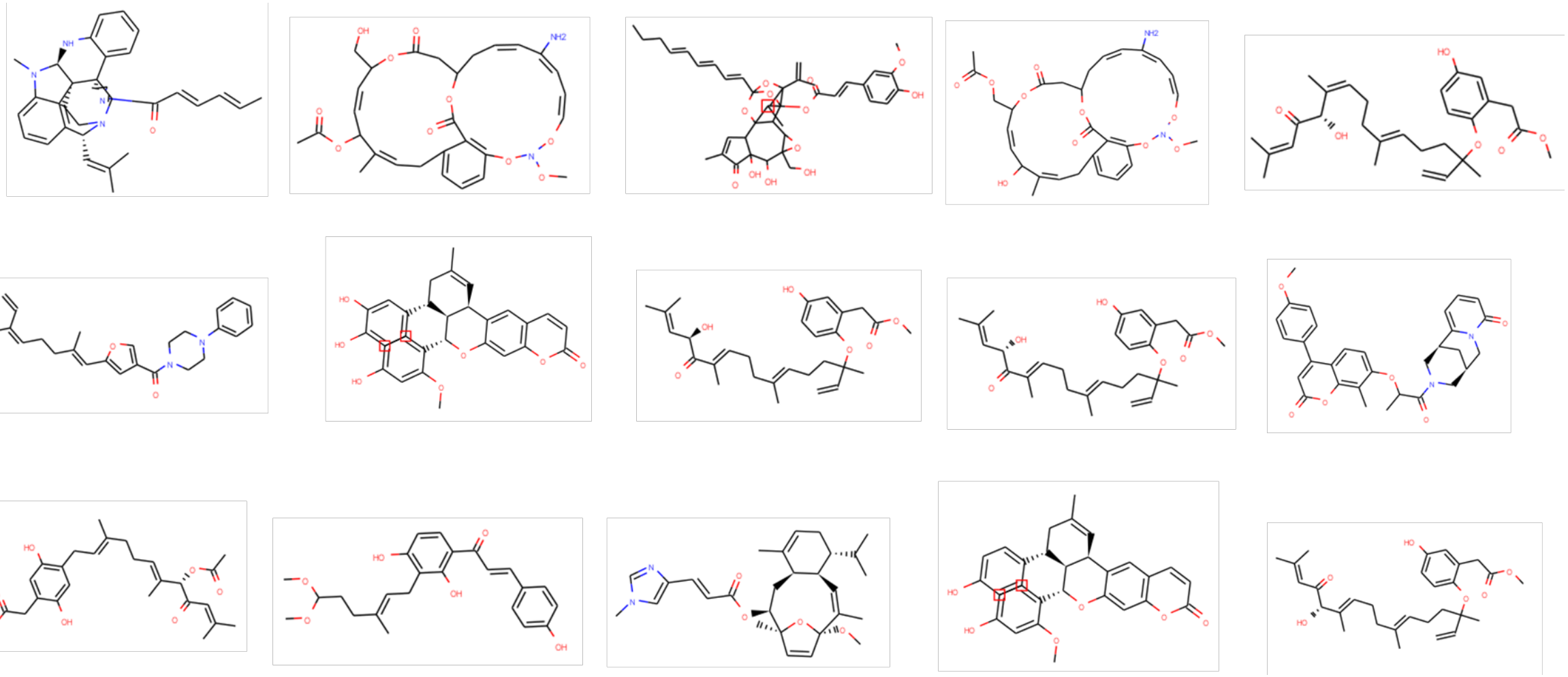


Figure S6. The structures of compounds predicted for sub-fraction E2-5 using SMART 2.0

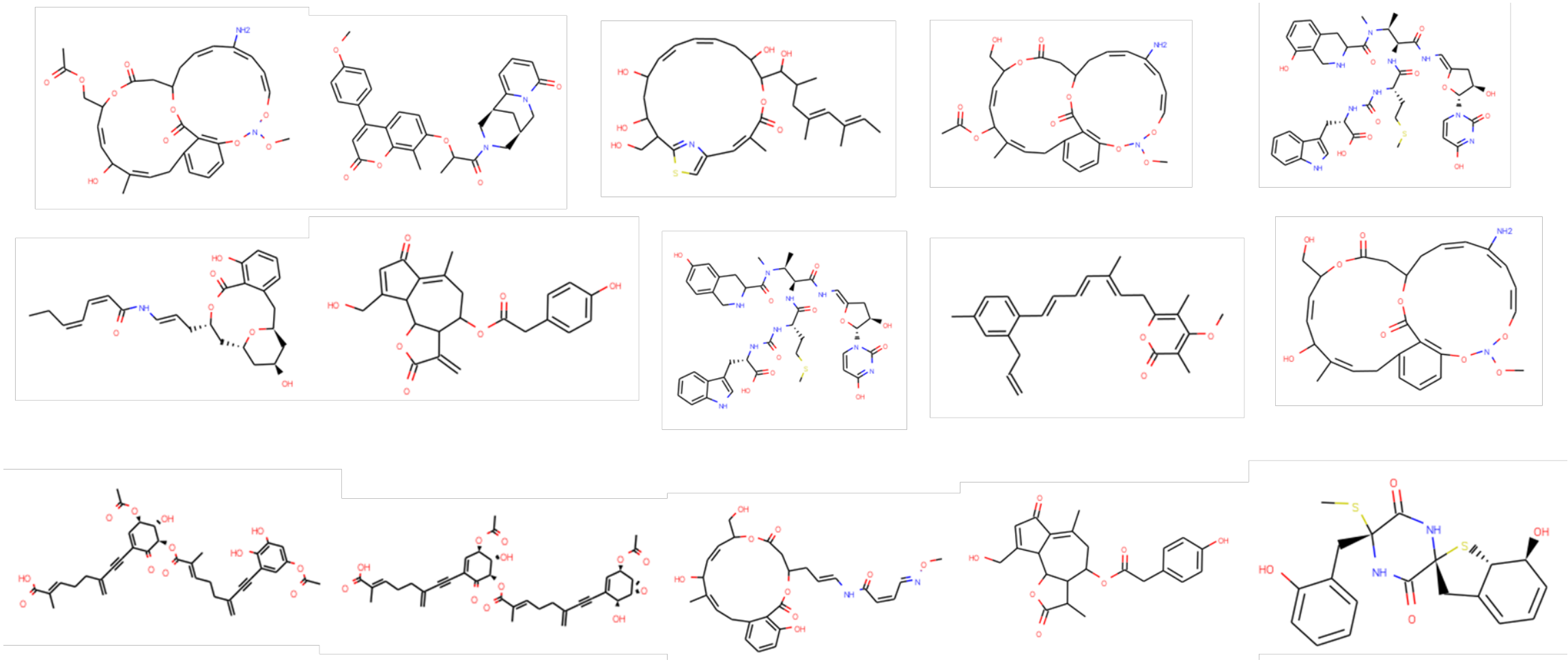


Figure S7. The structures of compounds predicted for sub-fraction E2-7 using SMART 2.0

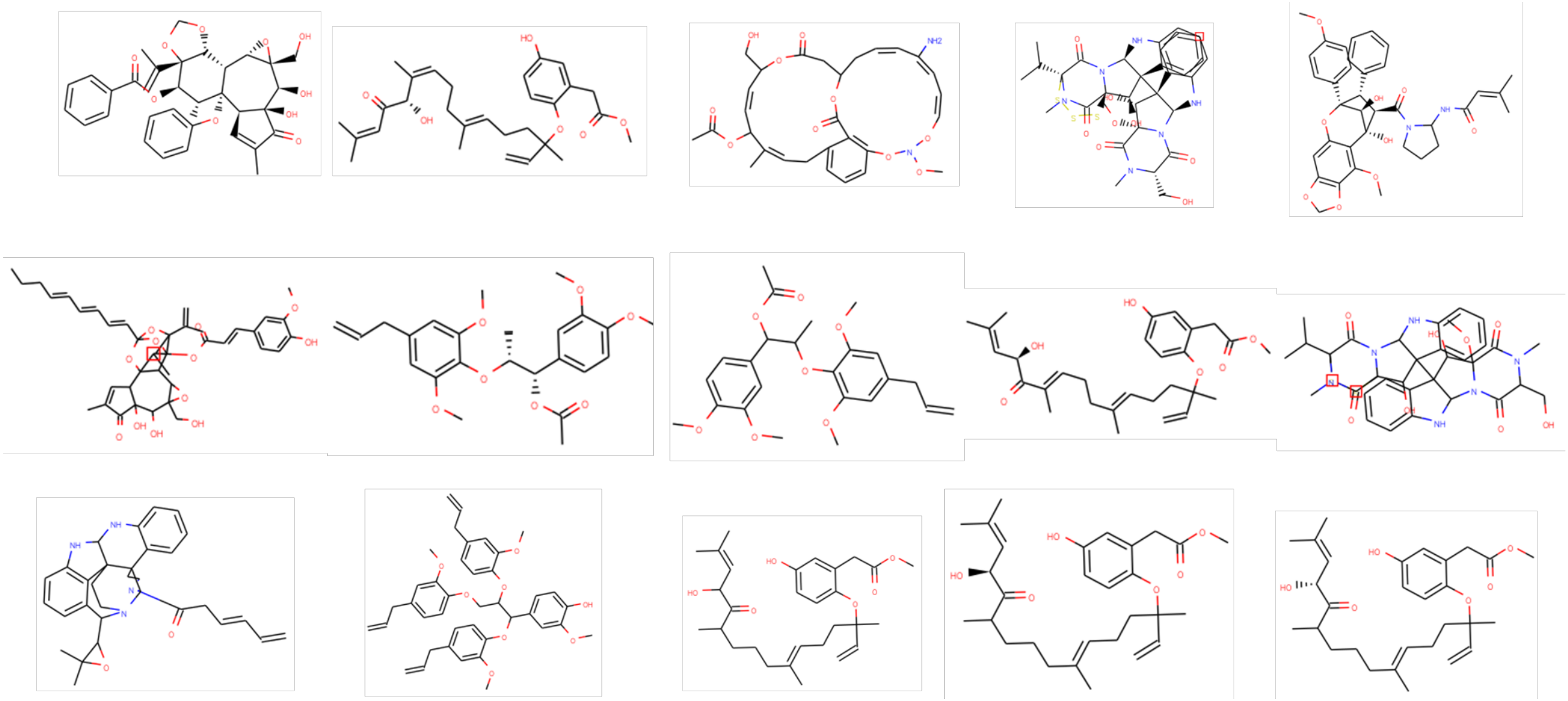


Figure S8. The ^{1}H NMR spectrum of **1** (CD_3OD, 600 MHz)

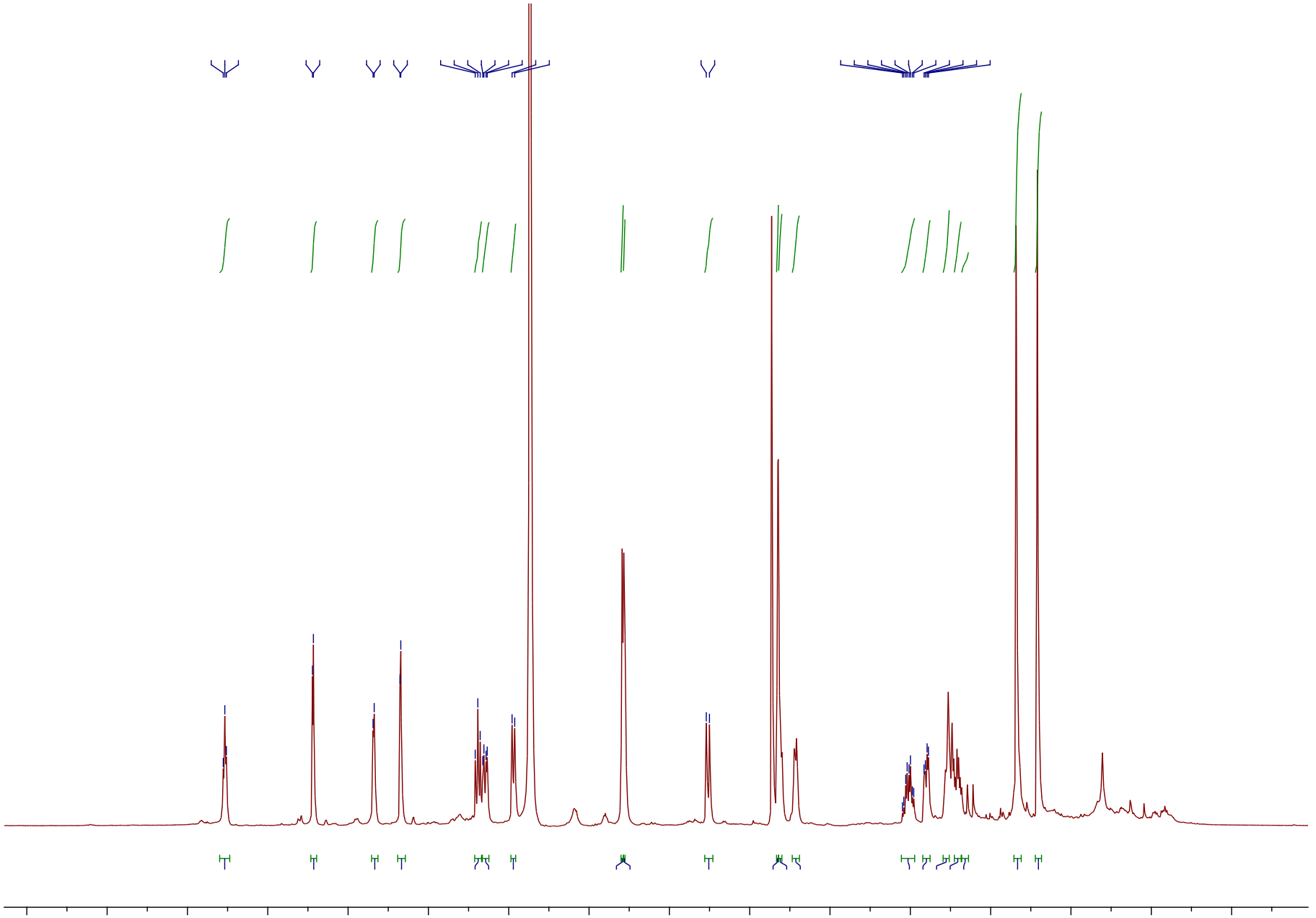


Figure S9. The ^{13}C NMR spectrum of **1** (CD_3OD, 150 MHz)

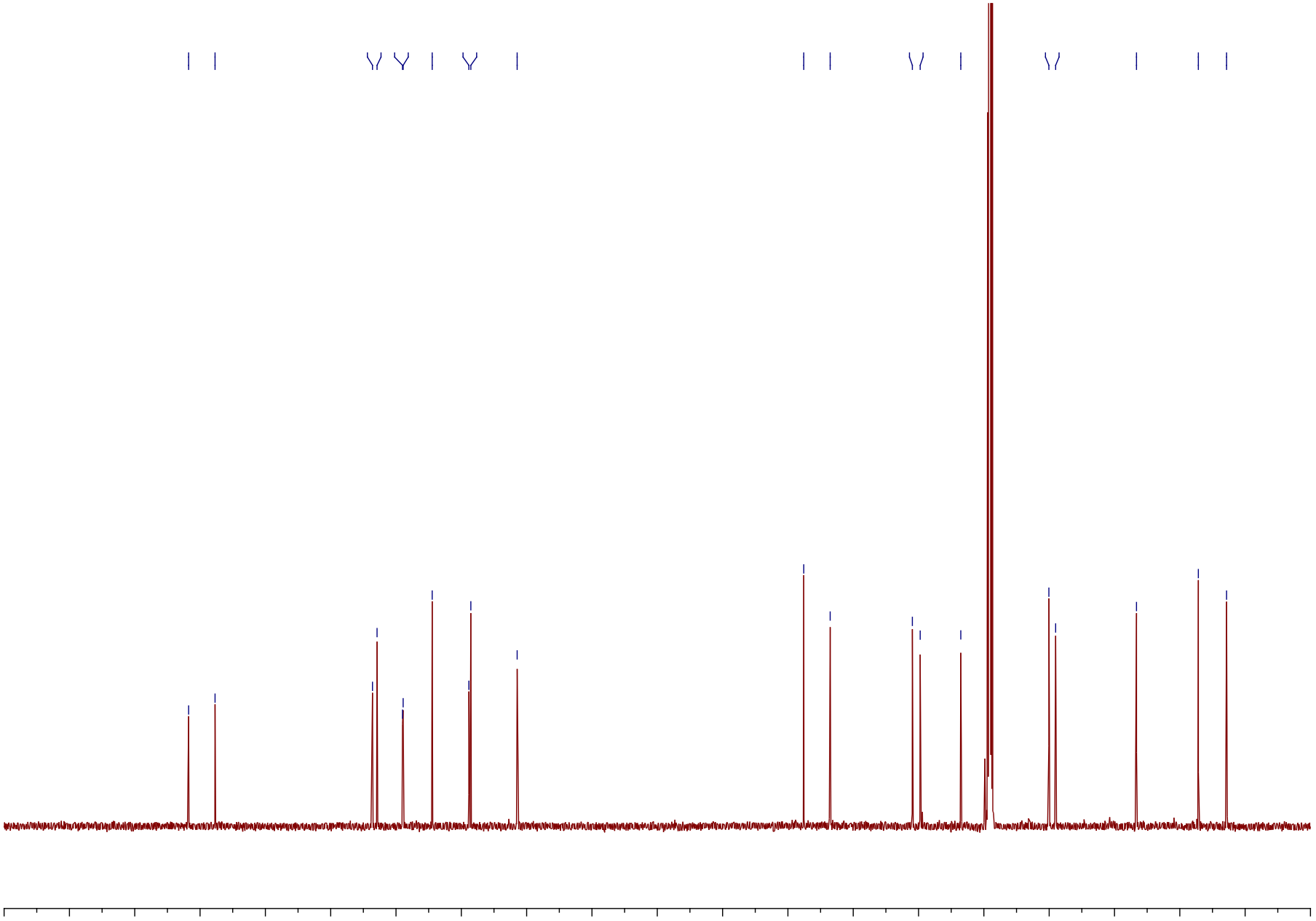


Figure S10. The HSQC spectrum of **1** (CD_3OD)

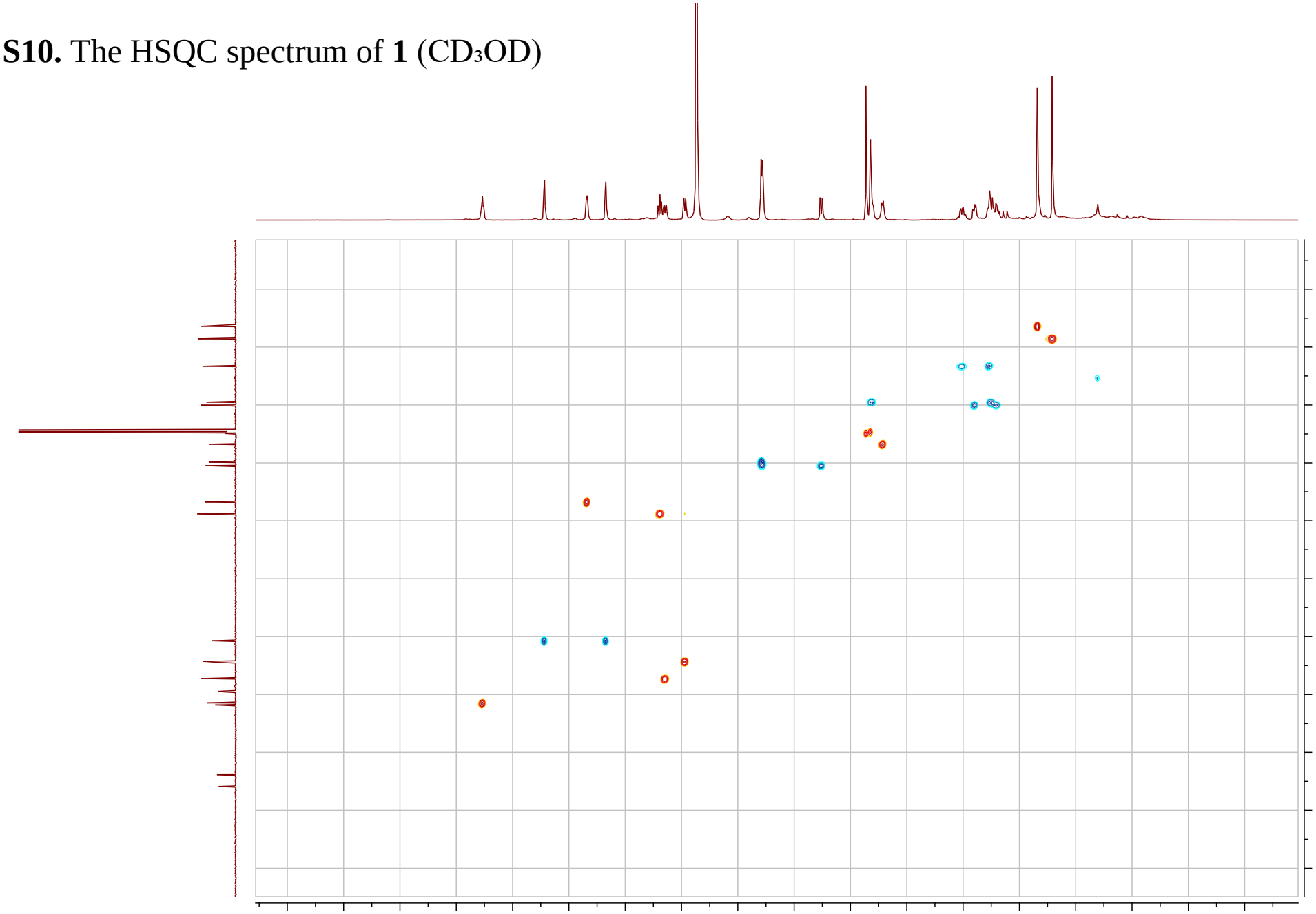


Figure S11. The ^{1}H-^{1}H COSY spectrum of **1** (CD_3OD)

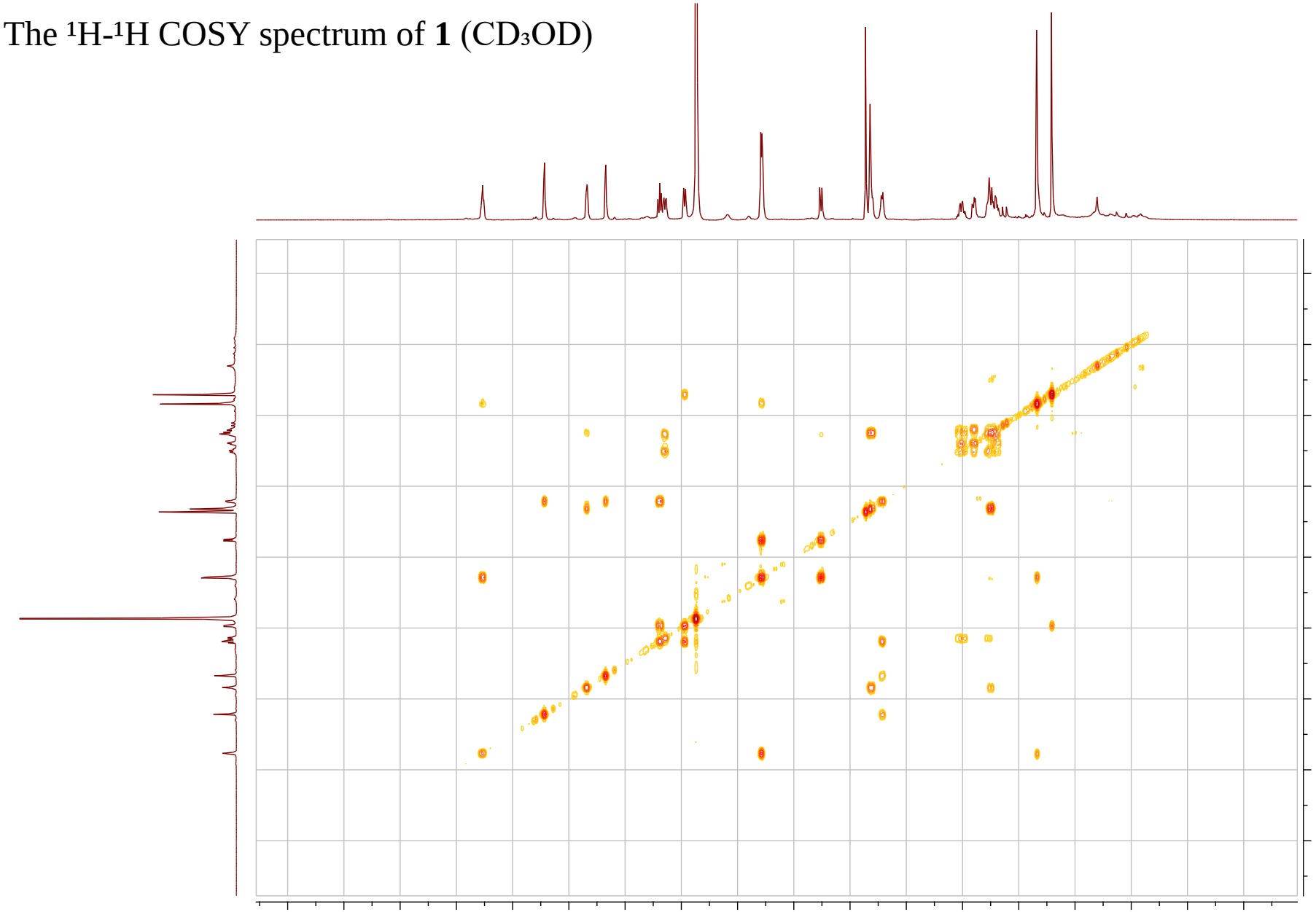


Figure S12. The HMBC spectrum of **1** (CD_3OD)

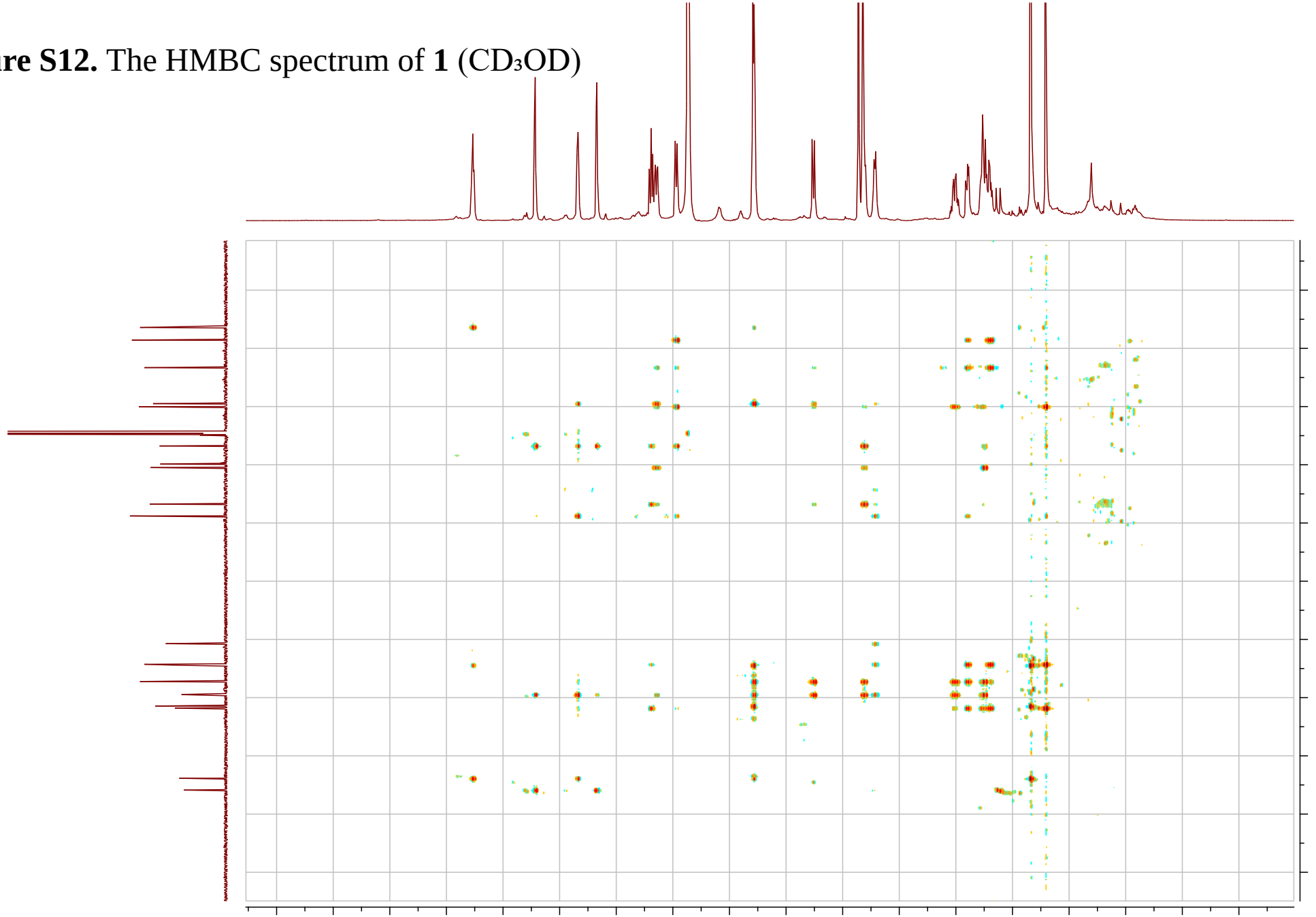
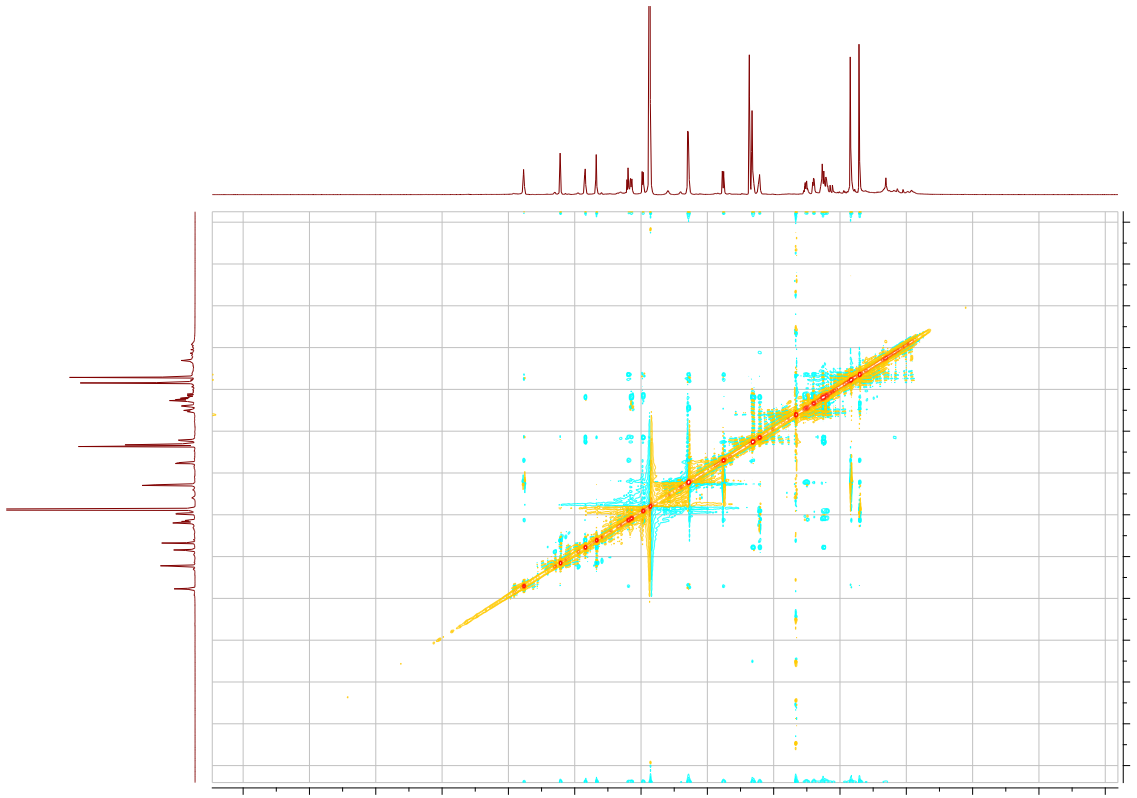


Figure S13. The ROESY spectrum of **1** (CD_3OD)



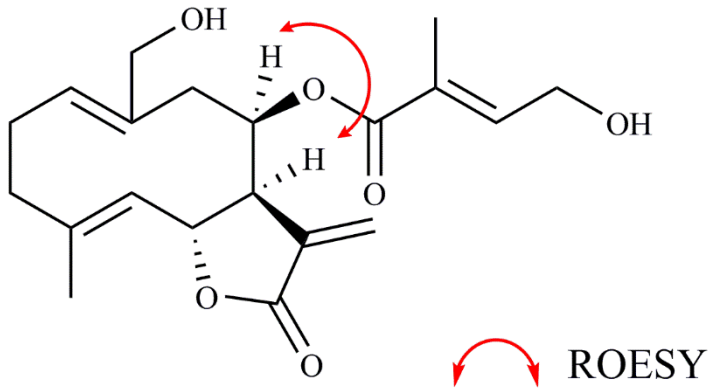


Table S1. Compounds from sub-fraction E2-4 predicted by SMART 2.0

Cosine score	Name
0.776	communesin J
0.774	aplidite E
0.740	acutilobin C
0.736	aplidite G
0.733	Methyl 2-[5-Hydroxy-2-[(6E,10Z,12S)-12-Hydroxy-3,7,11,15-Tetramethyl-13-Oxohexadeca-1,6,10,14-Tetraen-3-Yl]Oxyphenyl]Acetate
0.711	Not named
0.708	Palodesangren A
0.706	C29H40O6
0.706	C29H40O6
0.697	MLS001160351-01!
0.687	8'-acetoxyrietone
0.683	Xanthokeistal A
0.682	Methylcaribaeorane
0.681	Toddacoumalone
0.679	Palodesangren C

Table S2. Compounds from sub-fraction E2-5 predicted by SMART 2.0

Cosine score	Name
0.748	aplidite G
0.741	MLS001160351-01!
0.732	SCHEMBL10000000
0.724	aplidite E
0.720	CHEMBL3314791
0.714	apicularen A
0.710	Lactucopicrin
0.702	CHEMBL3314792
0.702	gombapyrone D
0.701	aplidite D
0.699	Tricholomenyn E
0.697	Tricholomenyn D
0.693	lobatamide D
0.690	Dihydro-lactucopicrin
0.688	eutypellazine O

Table S3. Compounds from sub-fraction E2-7 predicted by SMART 2.0

Cosine score	Name
0.747	Genkwadaphnin
0.720	Methyl 2-[5-Hydroxy-2-[(6E,10Z,12S)-12-Hydroxy-3,7,11,15-Tetramethyl-13-Oxohexadeca-1,6,10,14-Tetraen-3-Yl]Oxyphenyl]Acetate
0.692	aplidite E
0.690	Leptosin N1
0.687	19,20-Dehydroedulirin A
0.680	acutilobin C
0.680	(+)-Erythro-(7S,8R)-Delta8'-7-Acetoxy-3,4,3',5'-Tetramethoxy-8-O-4'-Neolignan
0.680	NCGC00380996-01![1-(3,4-dimethoxyphenyl)-2-(2,6-dimethoxy-4-prop-2-enylphenoxy)propyl] acetate
0.674	C29H40O6
0.674	C29H40O6
0.667	Leptosin M1
0.664	Communesin C (identified trough in silico generated spectrum)
0.661	tulsinol E
0.657	nahocol-A
0.657	C29H42O6

Table S4. Sesquiterpene lactones from sub-fraction E2-6 predicted by SMART 2.0

Cosine score	Name
0.880	Eupaglehnin A
0.866	8alpha-(Z-2-methyl-4-acetoxybut-2-enoyloxy)-15-hydroxygermacra-1(10),E,4Z,11(13)-trien-12,6alpha-olide
0.851	EUPACUNOLIN(Calcd_CDCl3)
0.838	15-isobutyrylmiguanin
0.833	Eupaglehnin B
0.824	vernangulide A
0.819	eupakirunsin B
0.817	2alpha-acetoxy-15-isovalerylmiguanin
0.811	Eupaglehnin C
0.805	Eupaglehnin D
0.799	melampolide 8
0.799	9alpha,14-dihydroxy-15-isobutyryloxycostunolide
0.799	9alpha,14-dihydroxy-15-isobutyryloxycostunolide
0.796	CHEMBL481634(Calcd_CDCl3)
0.795	hiyodorilactone B
0.789	Nobilin(Calcd_CDCl3)
0.785	CHEMBL388763(Calcd_CDCl3)
0.784	DEACETYLOVATIFOLIN(Calcd_CDCl3)
0.783	eupachinilide H
0.780	14-hydroxy-15-(2-methylbutyryloxy)-9-oxomelampolide
0.780	14-hydroxy-15-(2-methylbutyryloxy)-9-oxomelampolide
0.770	Heliangin(Calcd_CDCl3)
0.770	EUPACHINILIDE A(Calcd_CDCl3)
0.769	eupachinilide A