SUPPLEMENTARY MATERIAL

Narciclasine-4-*O*-*β*-D-xylopyranoside, a new narciclasine glycoside from *Zephyranthes minuta*

Deepali Katoch[ab*], Dharmesh Kumar[c], Yogendra S Padwad[ac], Bikram Singh[ab*], Upendra Sharma[ab*]

[a]*Academy of Scientific & Innovative Research, New Delhi, India*

[b]*Natural Product Chemistry and Process Development Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur, Himachal Pradesh 176061, India*

[c]*Department of Food and Nutraceuticals, CSIR-Institute of Himalayan Bioresource Technology, Palampur, Himachal Pradesh 176061, India*

ABSTRACT

A new narciclasine glycoside, narciclasine-4-*O*-*β*-D-xylopyranoside (**1**) was characterised along with four known alkaloids pancratistatin (**2**), 1-*O*-(3-hydroxybutyryl) pancratistatin (**3**), vittatine (**4**), 9-*O*-demethylgalanthine (**5**) from *Zephyranthes minuta*. Their structures were established on the basis of spectroscopic data analysis. The *in vitro* cytotoxic study of extract, fractions and isolated compounds against two human cancer cell lines (KB and SiHa) indicated the potential activity of extract and *n*-butanol fraction due to presence of active alkaloids pancratistatin, 1-*O*-(3-hydroxybutyryl) pancratistatin, lycorine and haemanthamine.

***Correspondence:** Dr. Bikram Singh, Dr. Upendra Sharma, Ms. Deepali Katoch, Natural Product Chemistry and Process Development Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur, Himachal Pradesh-176061, INDIA

E-mail: bikram_npp@rediffmail.com (bs); upendra@ihbt.res.in (us); deepalikatoch@outlook.com (dk)

Table 1: ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data for Compound 1 (δ in ppm) in MeOD-d_4 (J in Hz).

Position	δ_H (ppm)	δ_C (ppm)	DEPT
1	6.13, brs	123.8	CH
2	4.20, brs	70.3	CH
3	3.98, m*	72.0	CH
4	3.93, d*	79.6	CH
4a	4.34, d (J= 9.0 Hz)	52.0	CH
6	-	170.4	C
6a	-	107.1	C
7	-	146.5	C
8	-	135.8	C
9	-	154.4	C
10	6.70, s	97.3	CH
10a	-	132.1	C
10b	-	133.2	C
-O$\underline{C}$H$_2$O-	5.96, s	103.7	CH$_2$
1’	4.31, d (J= 7.6 Hz)	104.0	CH
2’	3.24, m*	74.8	CH
3’	3.30, m*	77.6	CH
4’	3.53, m	71.0	CH
5’	3.98, m*; 3.21, m*	67.2	CH$_2$

*overlapped signals

Table S2: IC_{50} values of extract, fractions and alkaloids against KB and SiHa cell lines.

Extract	IC_{50} (µg/mL) value for cell lines	
	KB	**SiHa**
Extract	184.25	<25
Fractions		
n-hexane	>200	>200
Chloroform	>200	111.88
n-butanol	54.34	<25
Water	>200	>200
Alkaloids	**IC_{50} (µM) value for cell lines**	
Narciclasine-4-*O*-*β*-D-xylopyranoside	>100	>100
Pancratistatin	<10	<10
1-*O*-(3-hydroxybutyryl) pancratistatin	18.27	<10
Vittatine	>100	>100
Hamayne	>100	>100
Haemanthamine	21.1	22.37
Lycorine	42.74	22.75
9-*O*-demethylgalanthine	>100	>100
Galanthine	>100	>100
Tortuosine	>100	>100
Ungeremine	>100	>100
Lycoramine	>100	>100

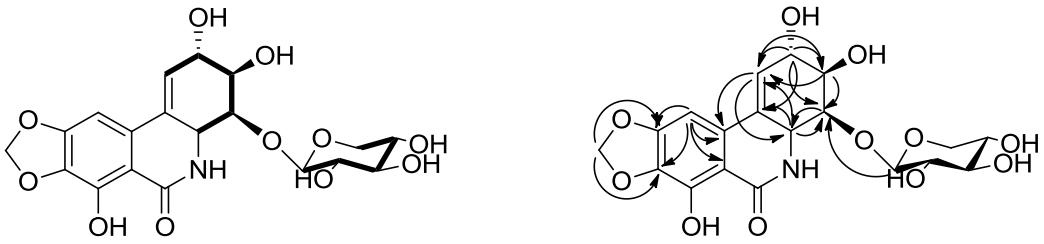

Figure S1. The ^{1}H-^{1}H COSY (——) and key HMBC correlations (H→C) of compound(1).

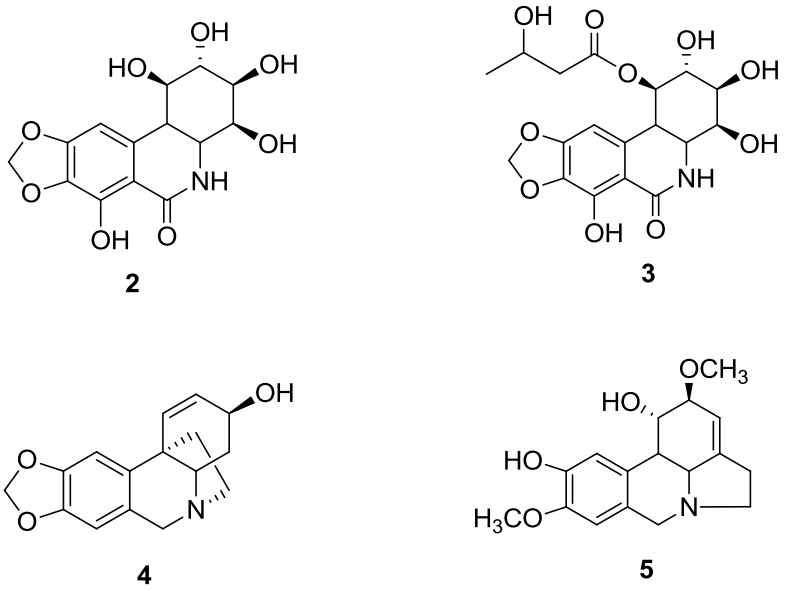

Figure S2. Structures of the isolated alkaloids (2-5).

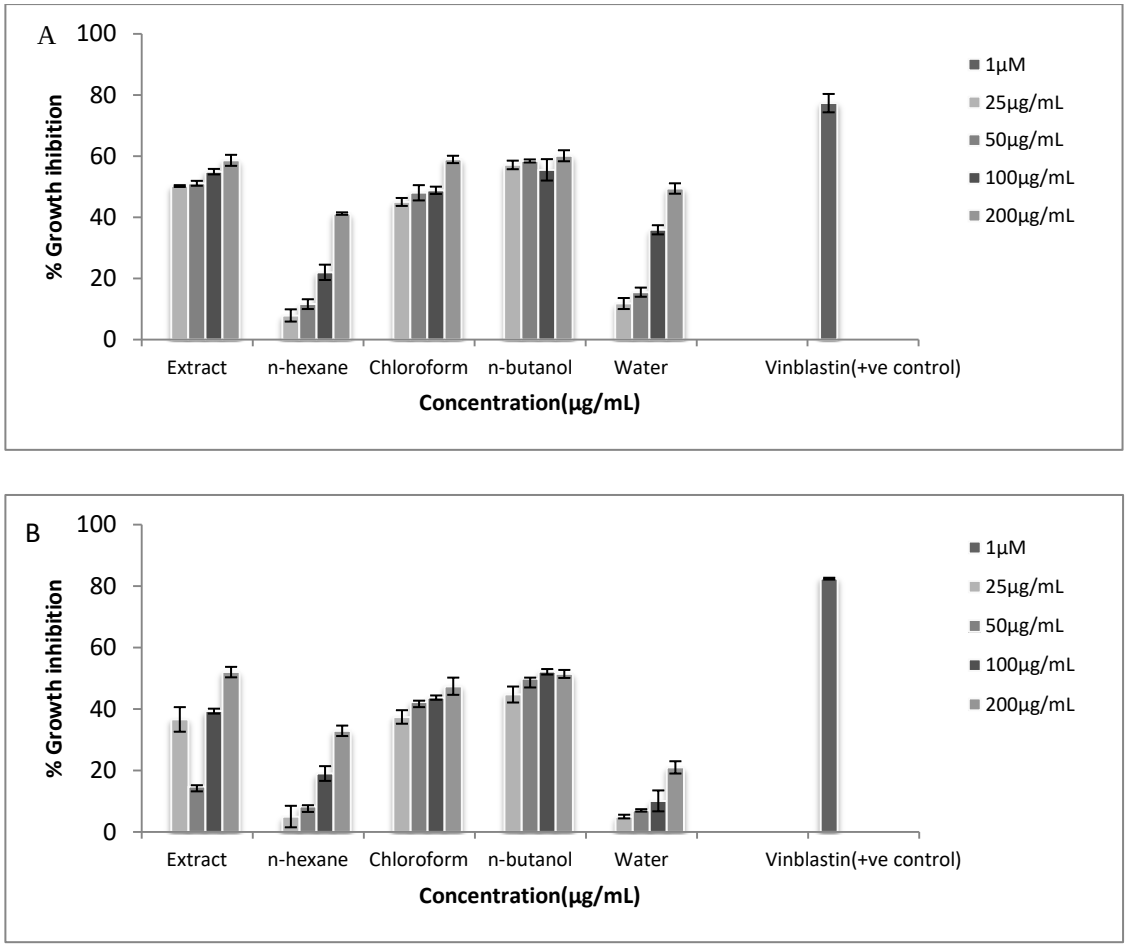

Figure S3: Growth inhibition by extract and fractions using SRB assay A. *In vitro* cytotoxicity against KB cell lines and B. *In vitro* cytotoxicity against SiHa cell lines

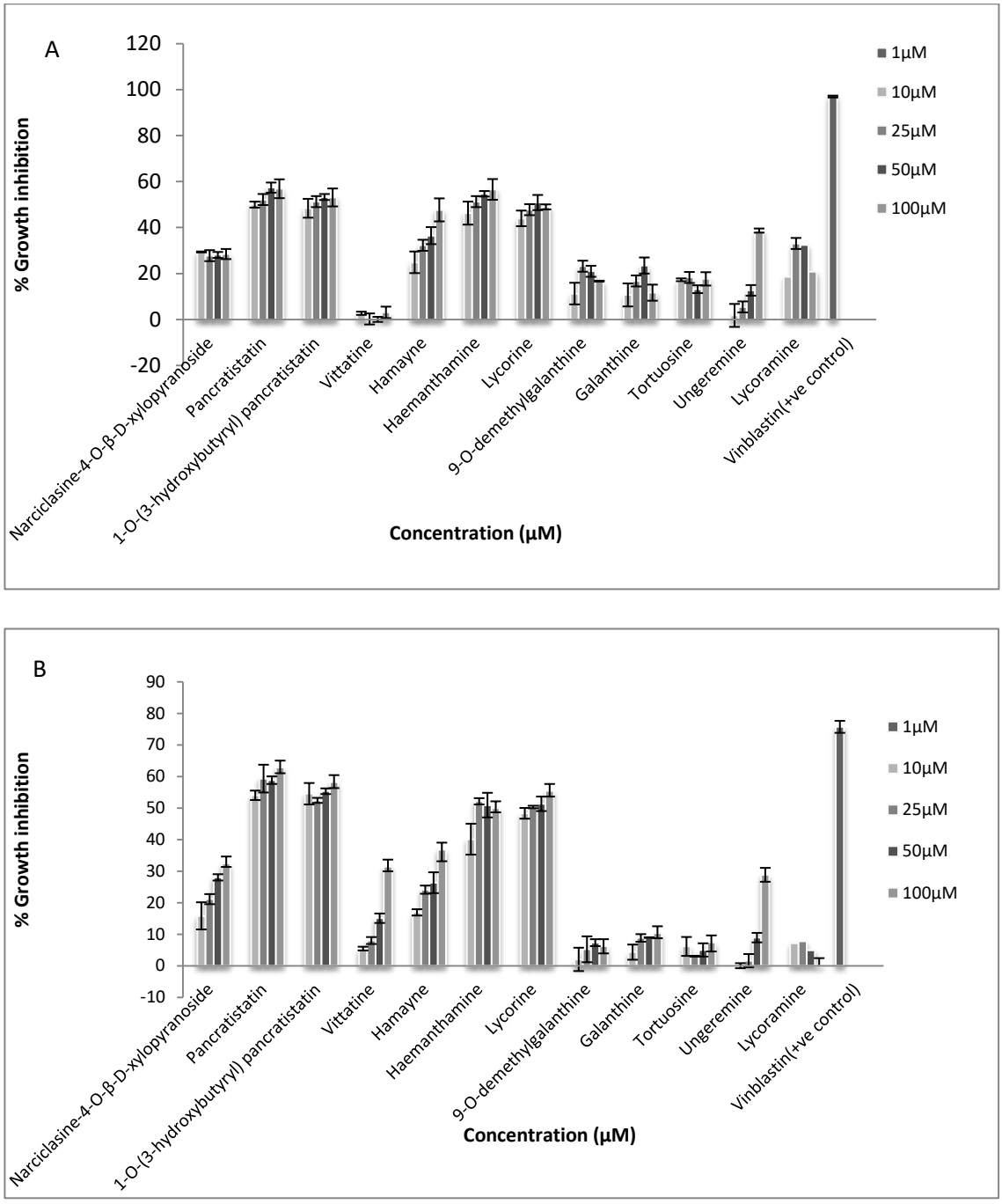

Figure S4: Growth inhibition by Amaryllidaceae alkaloids using SRB assay A. *In vitro* cytotoxicity against KB cell lines and B. *In vitro* cytotoxicity against SiHa cell lines

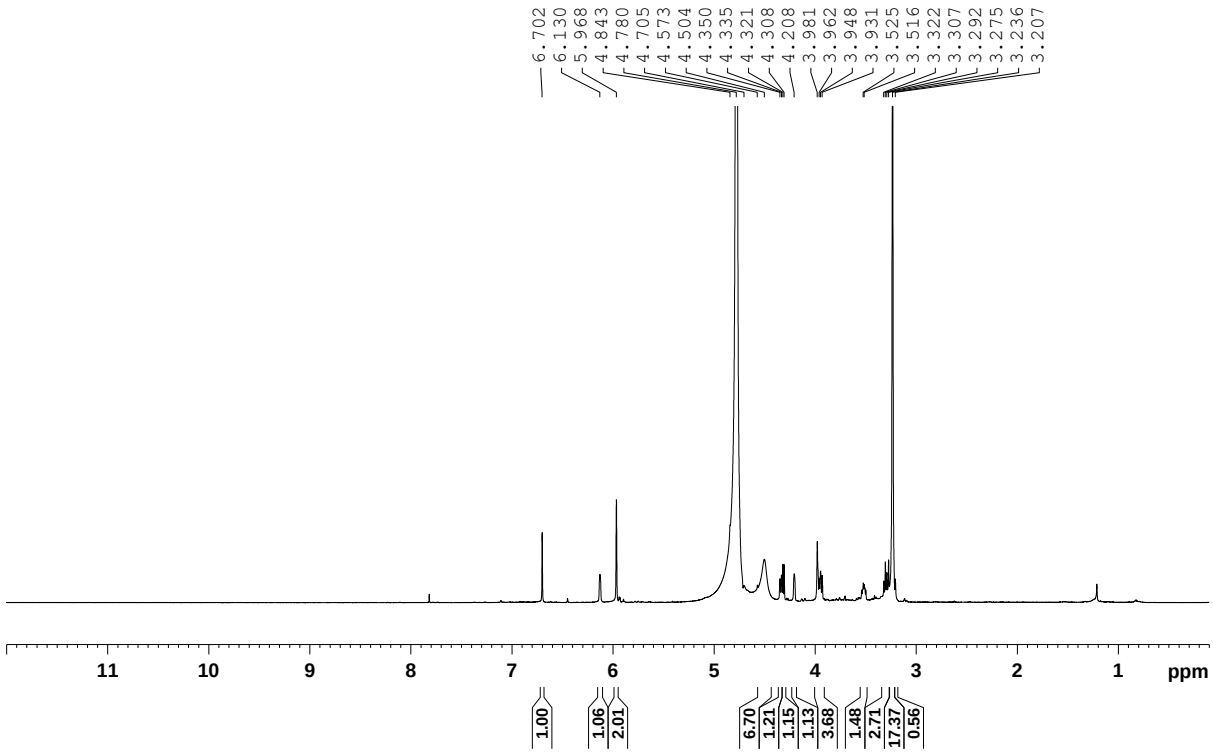

Figure S5. ^{1}H NMR spectrum for compound 1 in MeOD-d_4

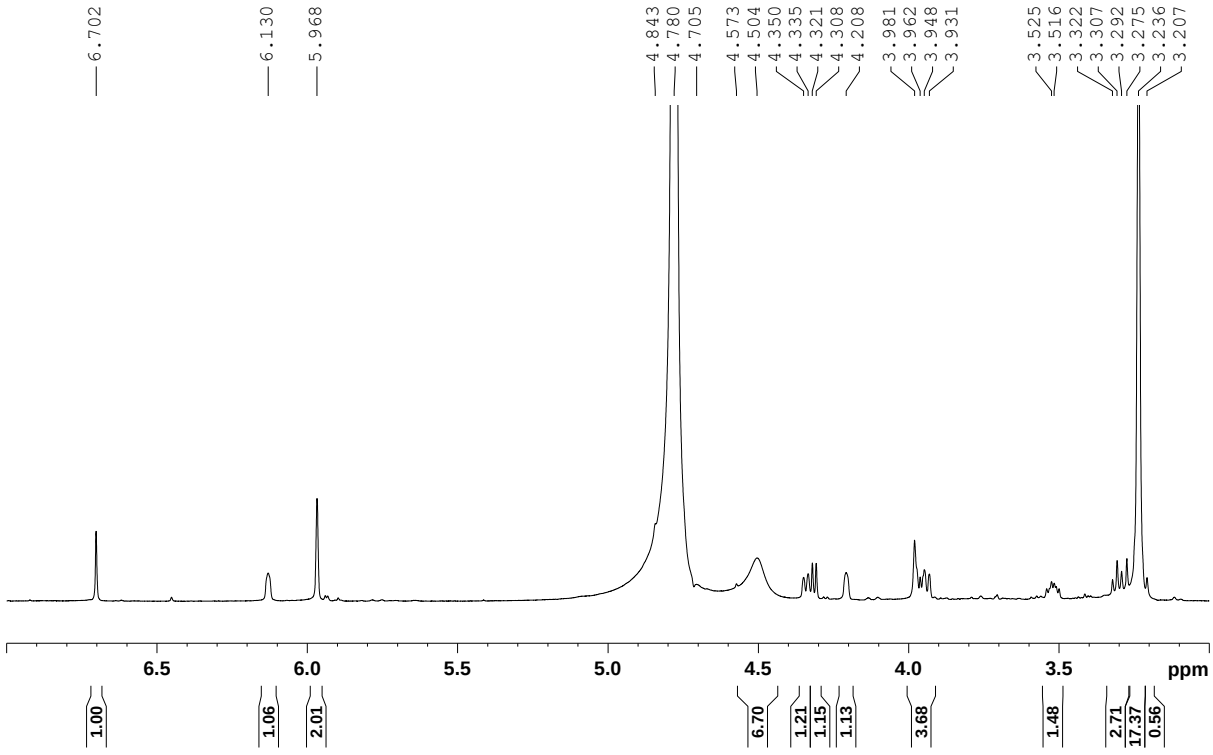

Figure S6. ^{1}H NMR spectrum expansion for compound 1 in MeOD-d_4

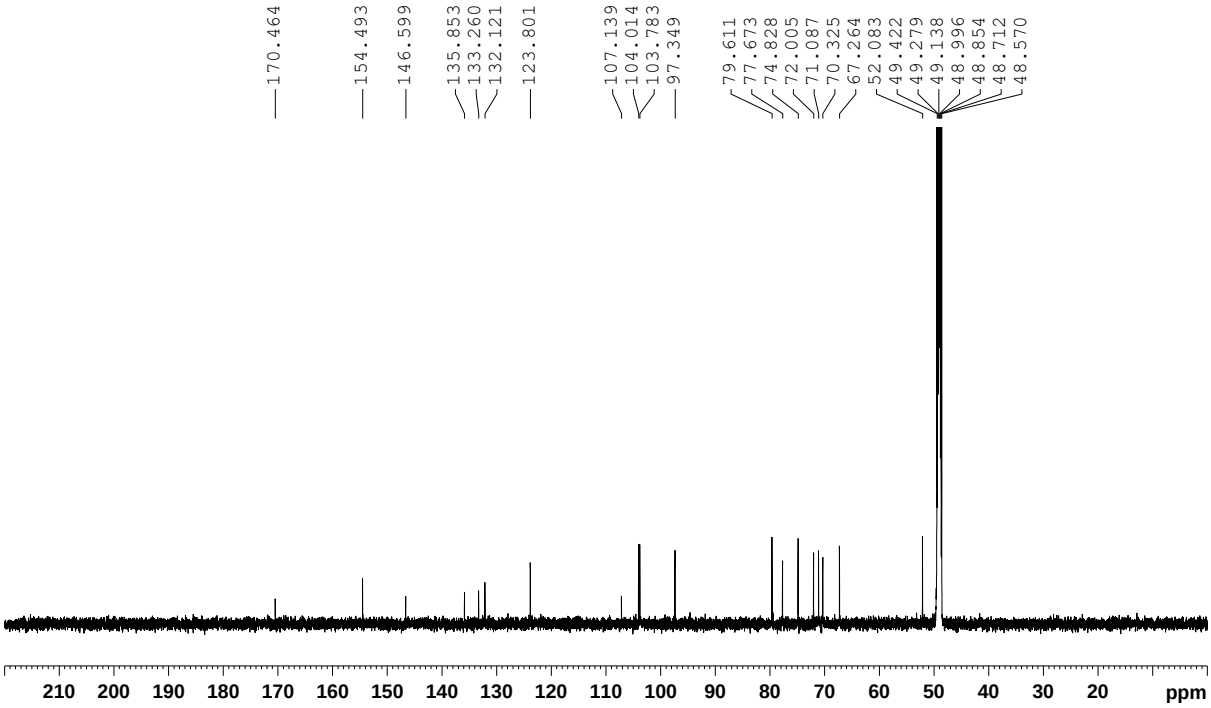

Figure S7. ^{13}C NMR spectrum for compound 1 in MeOD-d_4

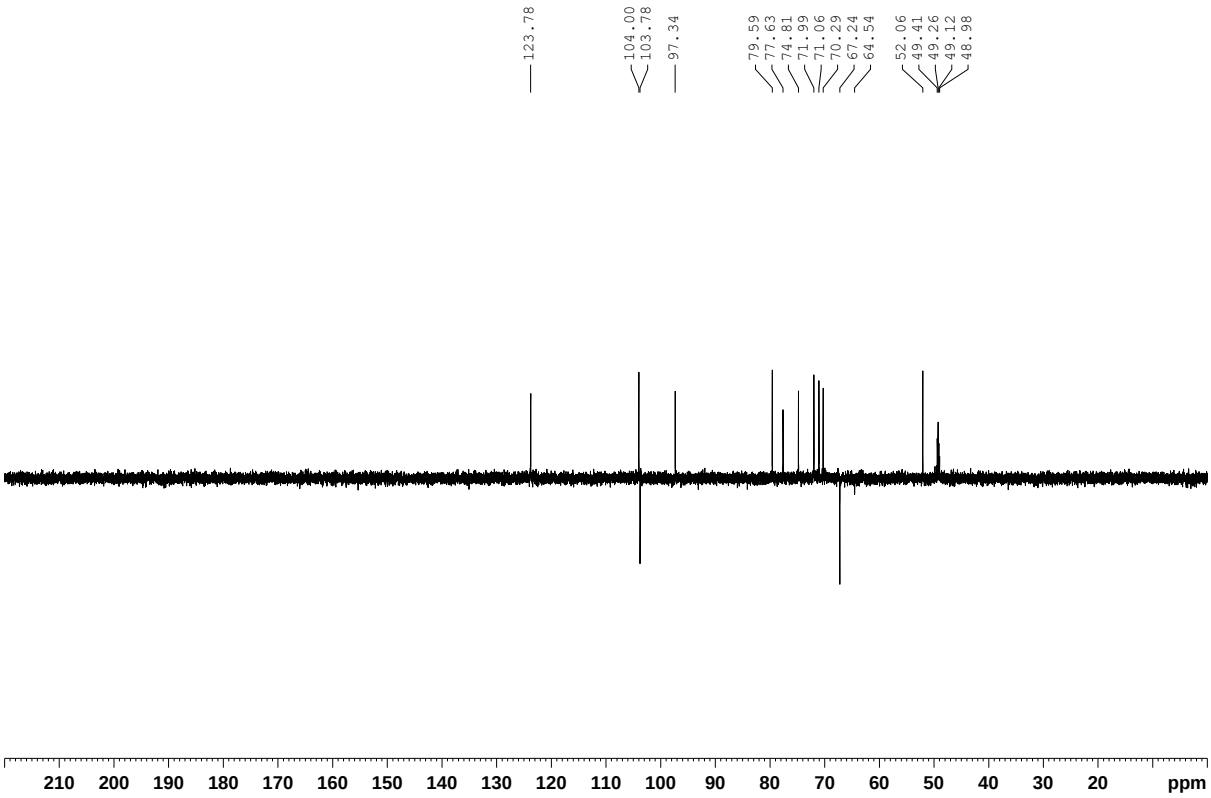

Figure S8. DEPT NMR spectrum for compound 1 in MeOD-d_4

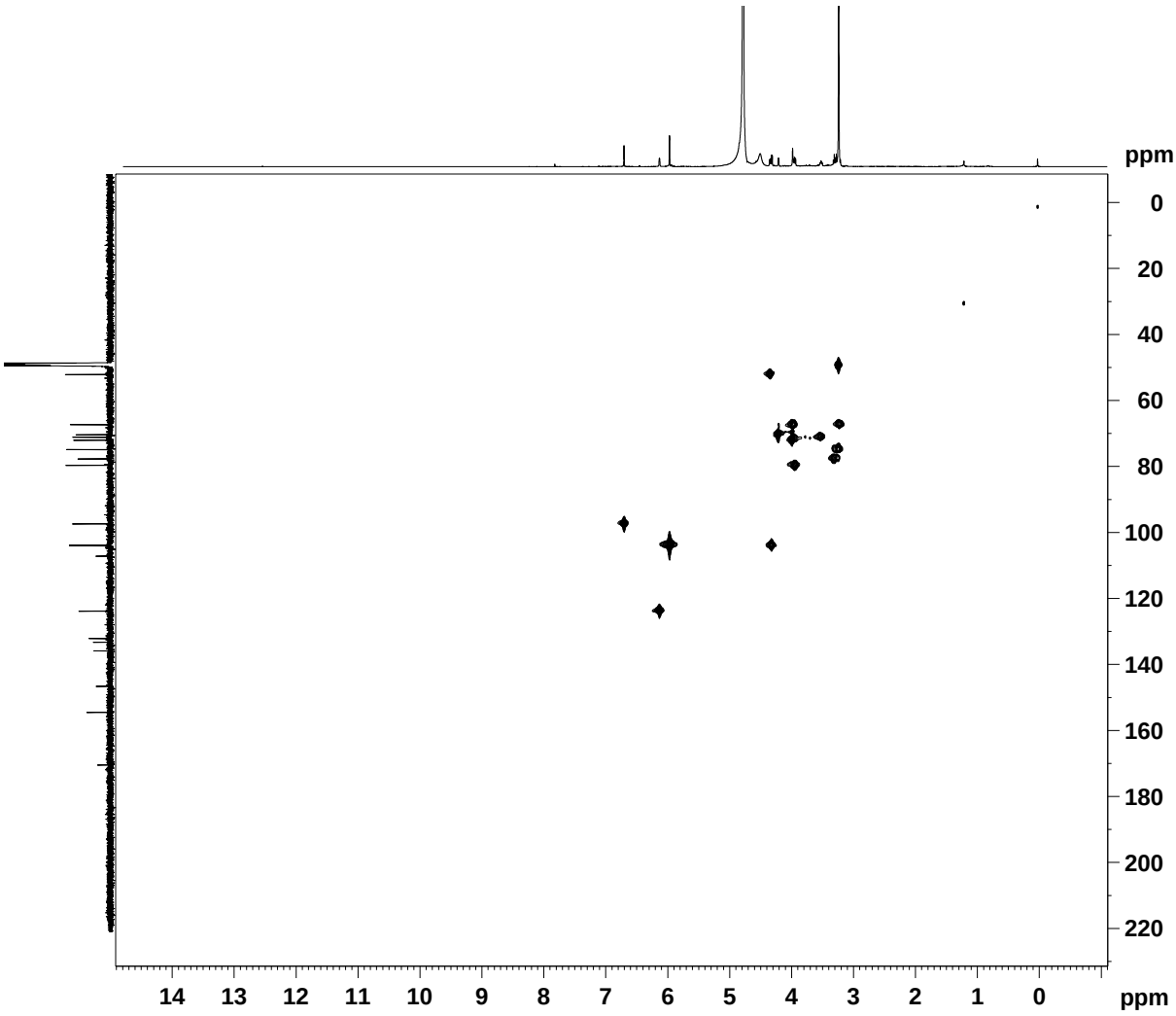

Figure S9. HMQC spectrum for compound 1 in MeOD-d_4

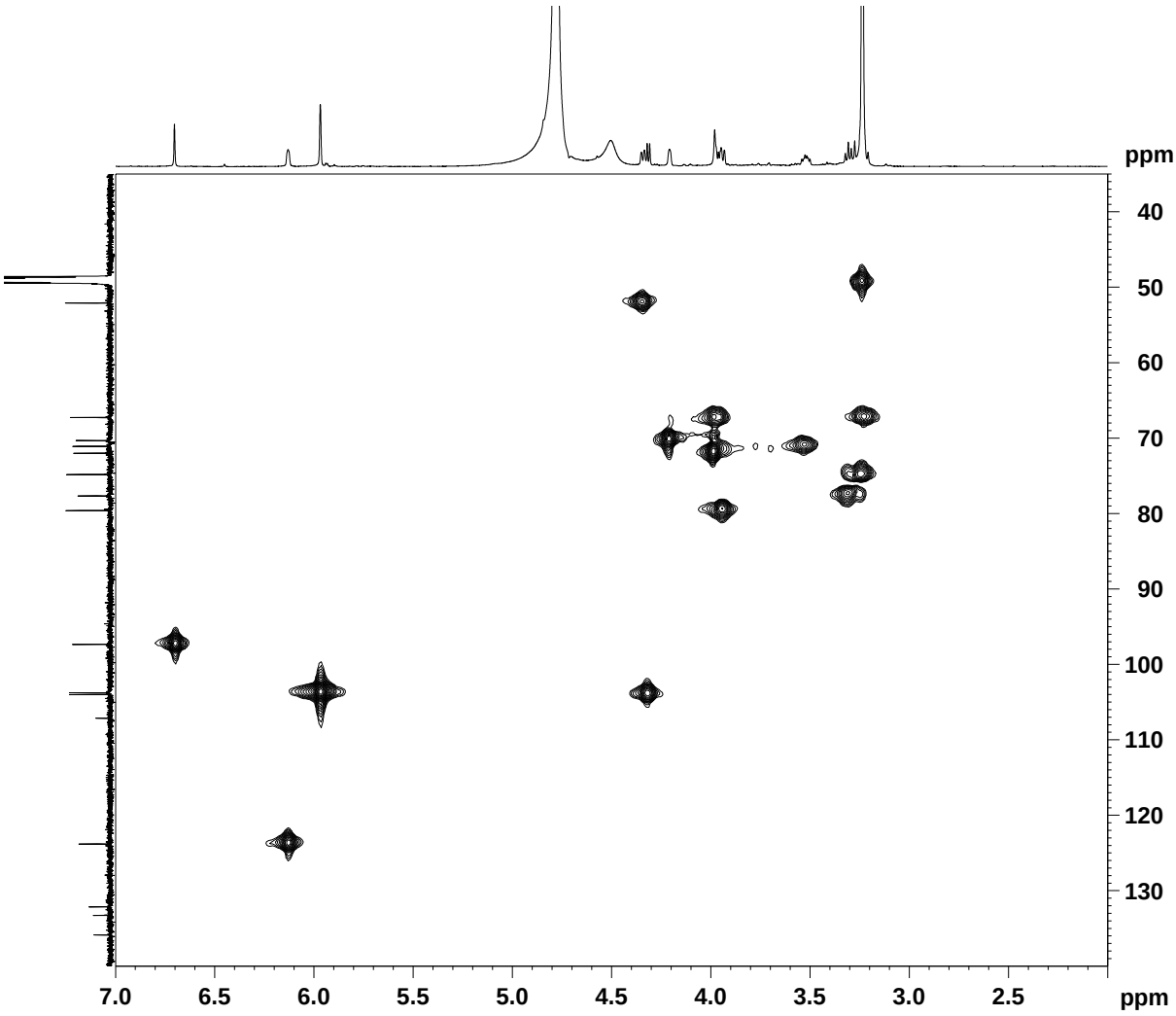

Figure S10. Expansion of the HMQC spectrum for compound 1

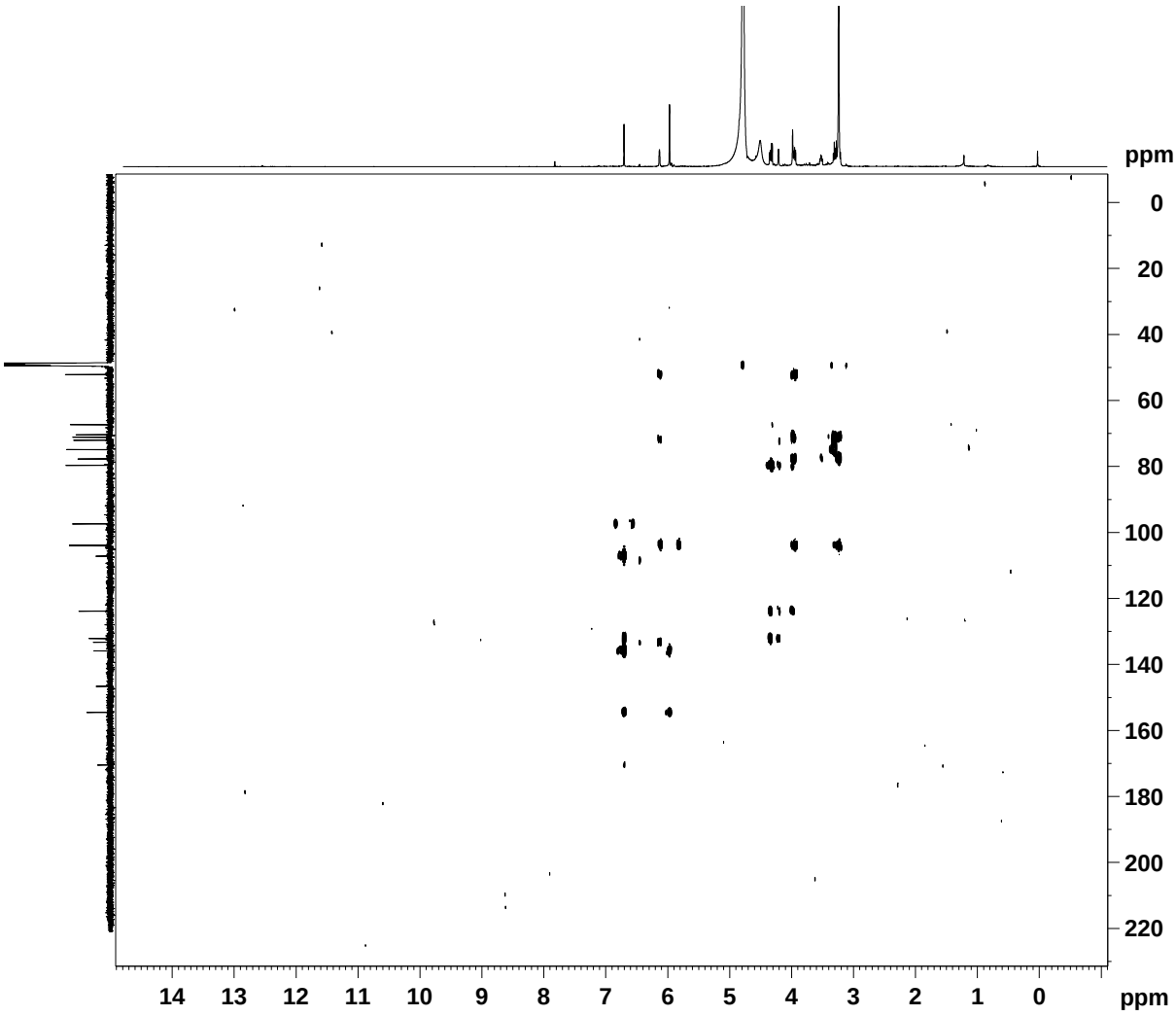

Figure S11. HMBC spectrum for compound 1 in MeOD-d_4

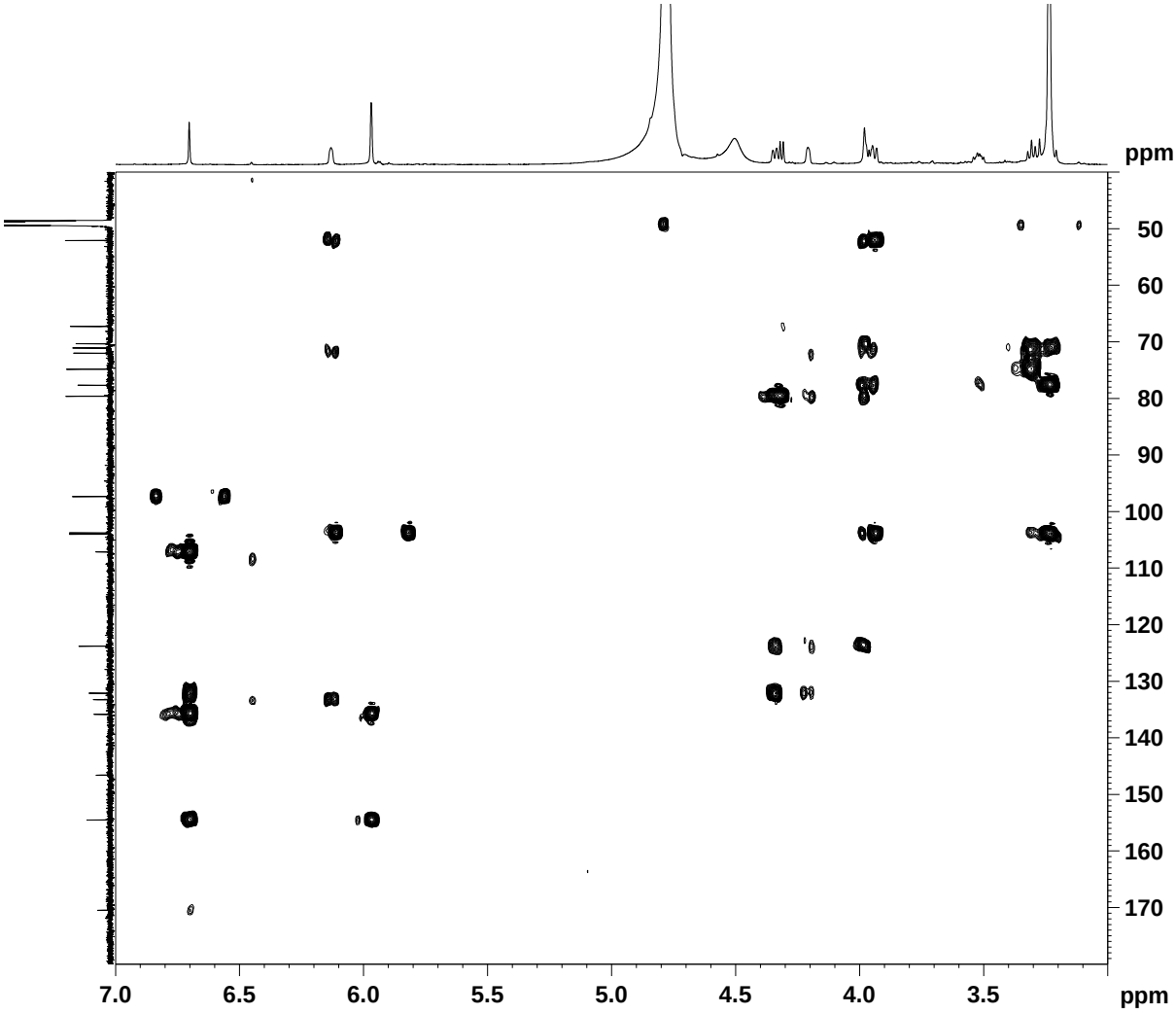

Figure S12. Expansion of the HMBC spectrum for compound 1

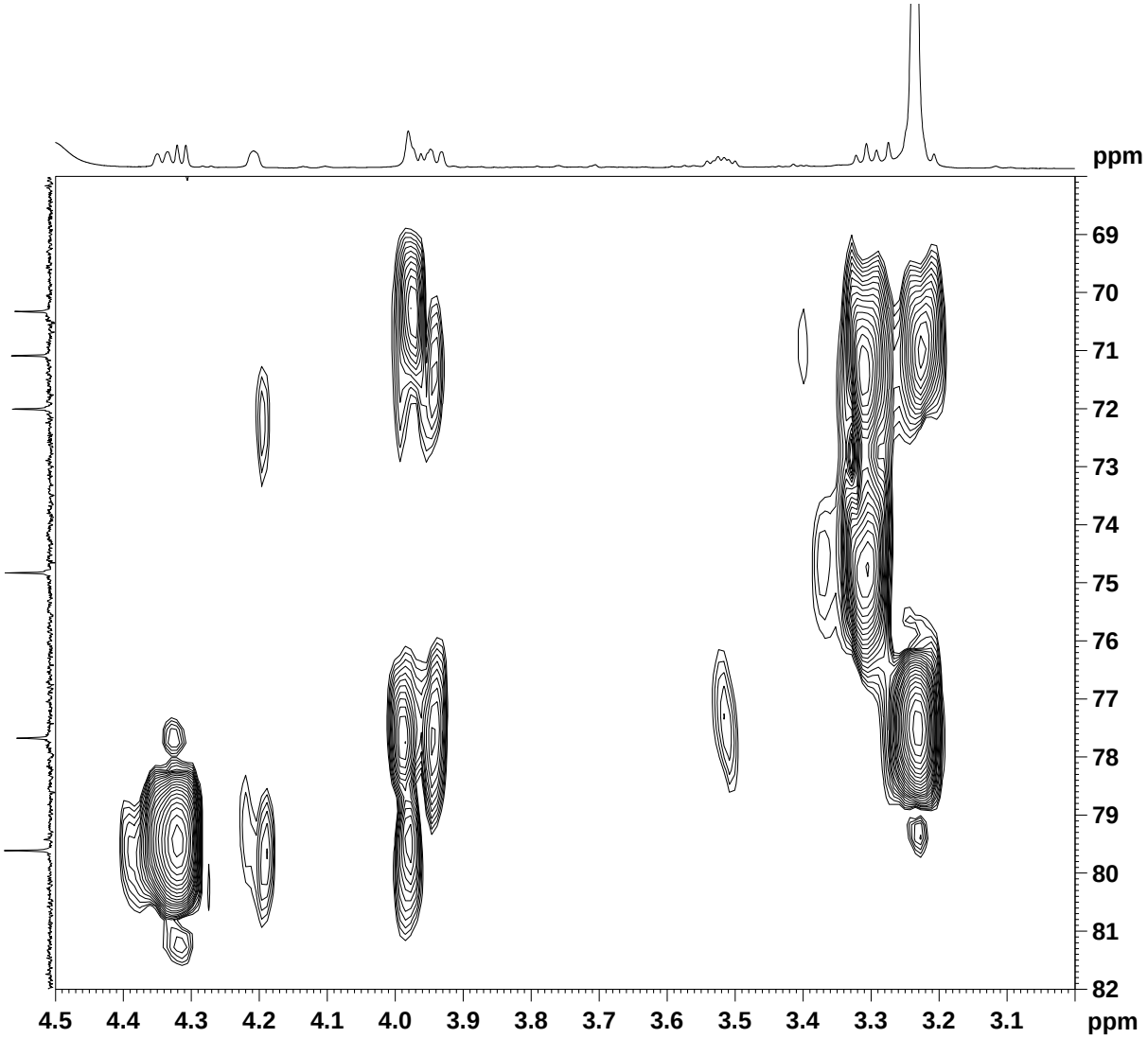

Figure S13. Expansion of the HMBC spectrum for compound 1(continued)

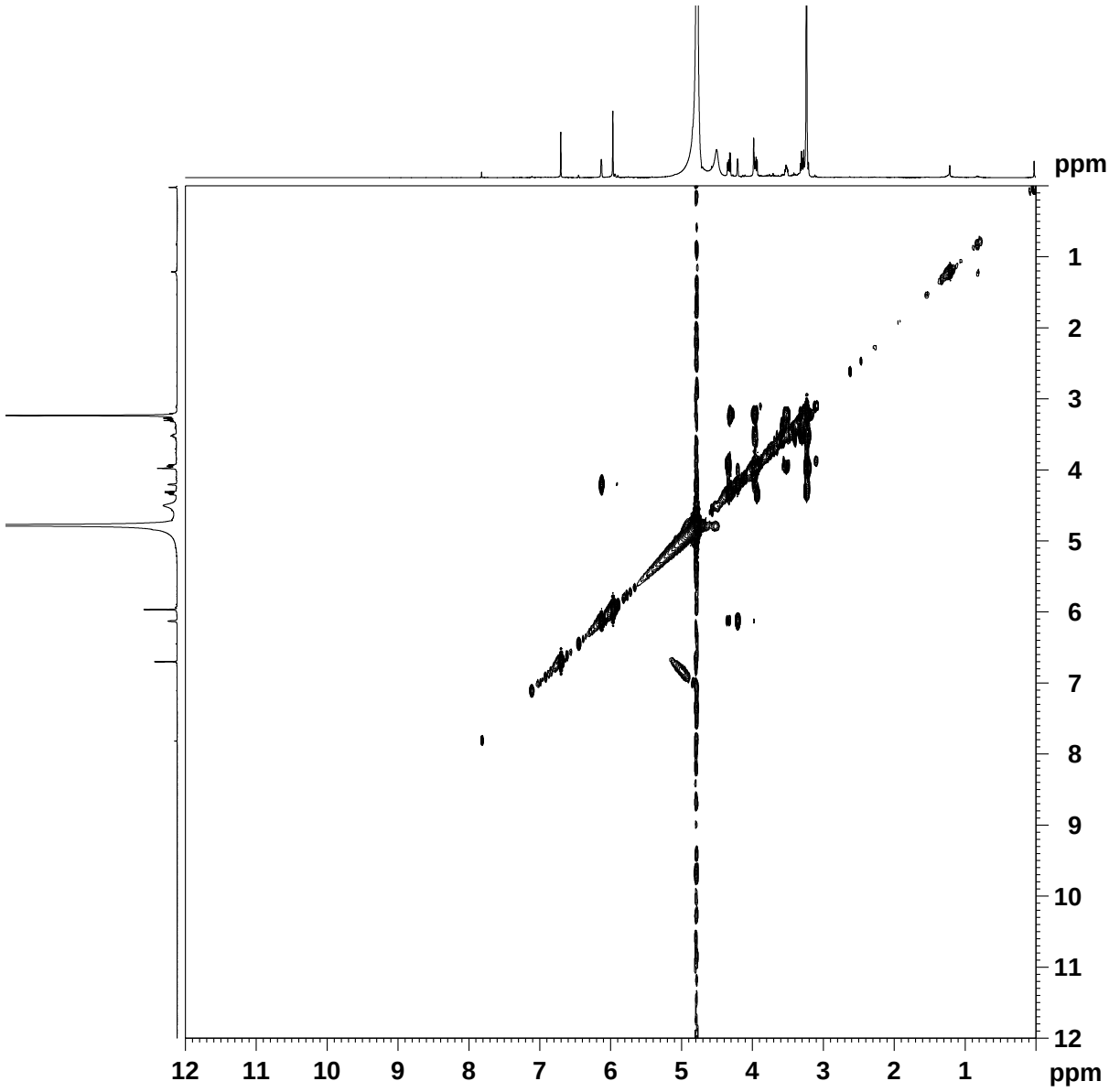

Figure S14. ^{1}H-^{1}H COSY spectrum for compound 1 in MeOD-d_4

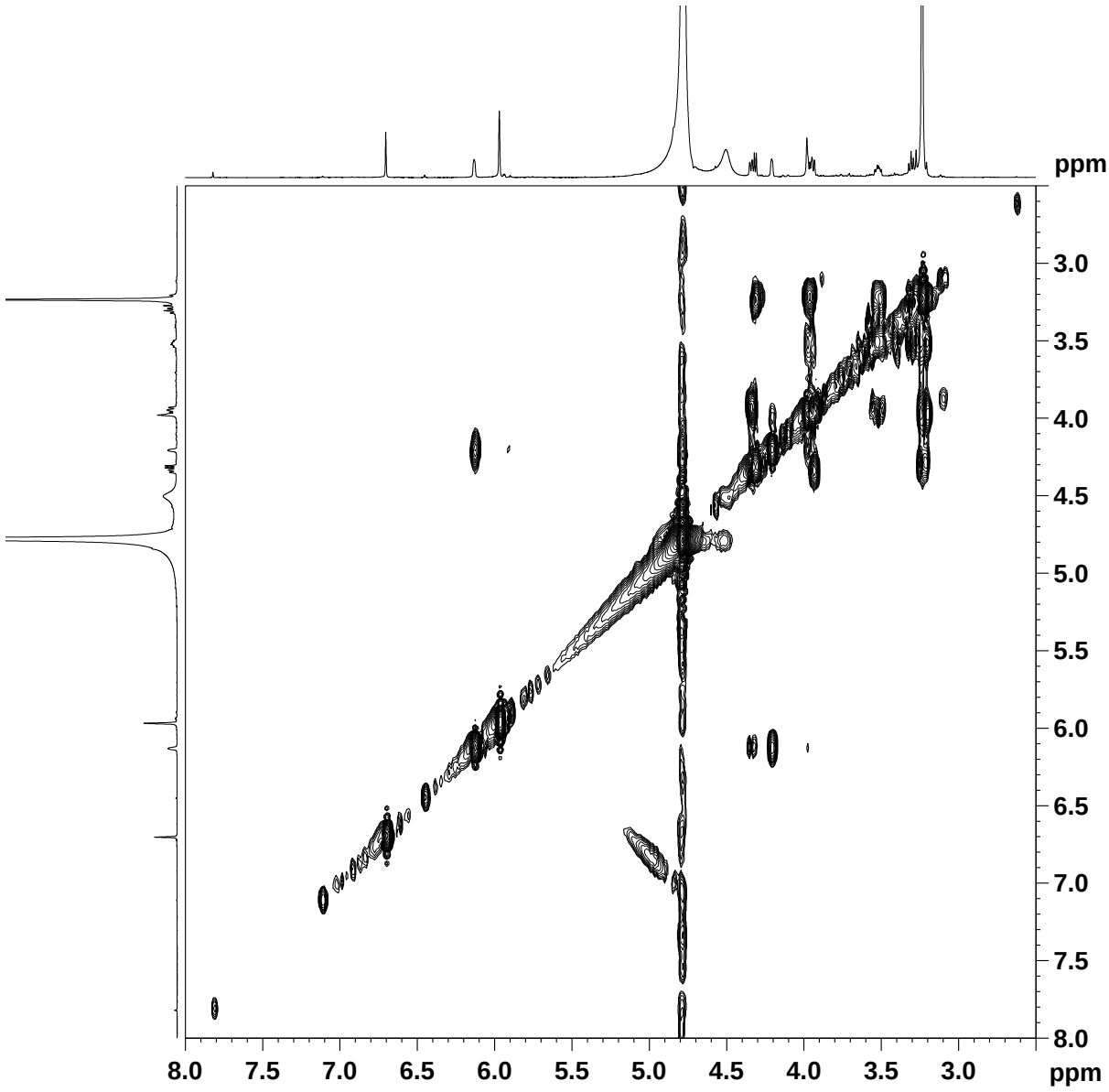

Figure S15. Expansion of ^{1}H-^{1}H COSY spectrum for compound 1

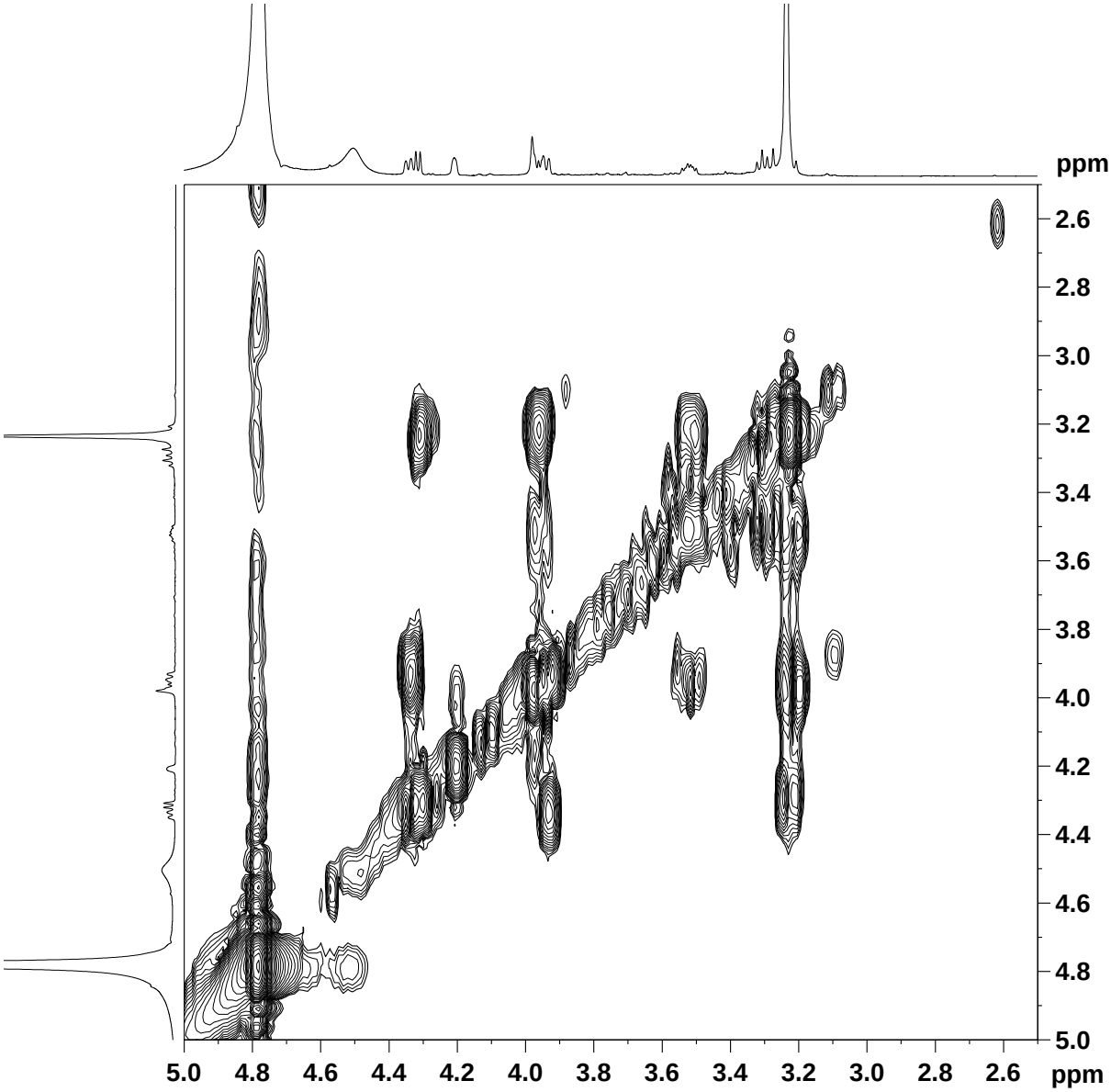

Figure S16. Expansion of ^{1}H-^{1}H COSY spectrum for compound 1

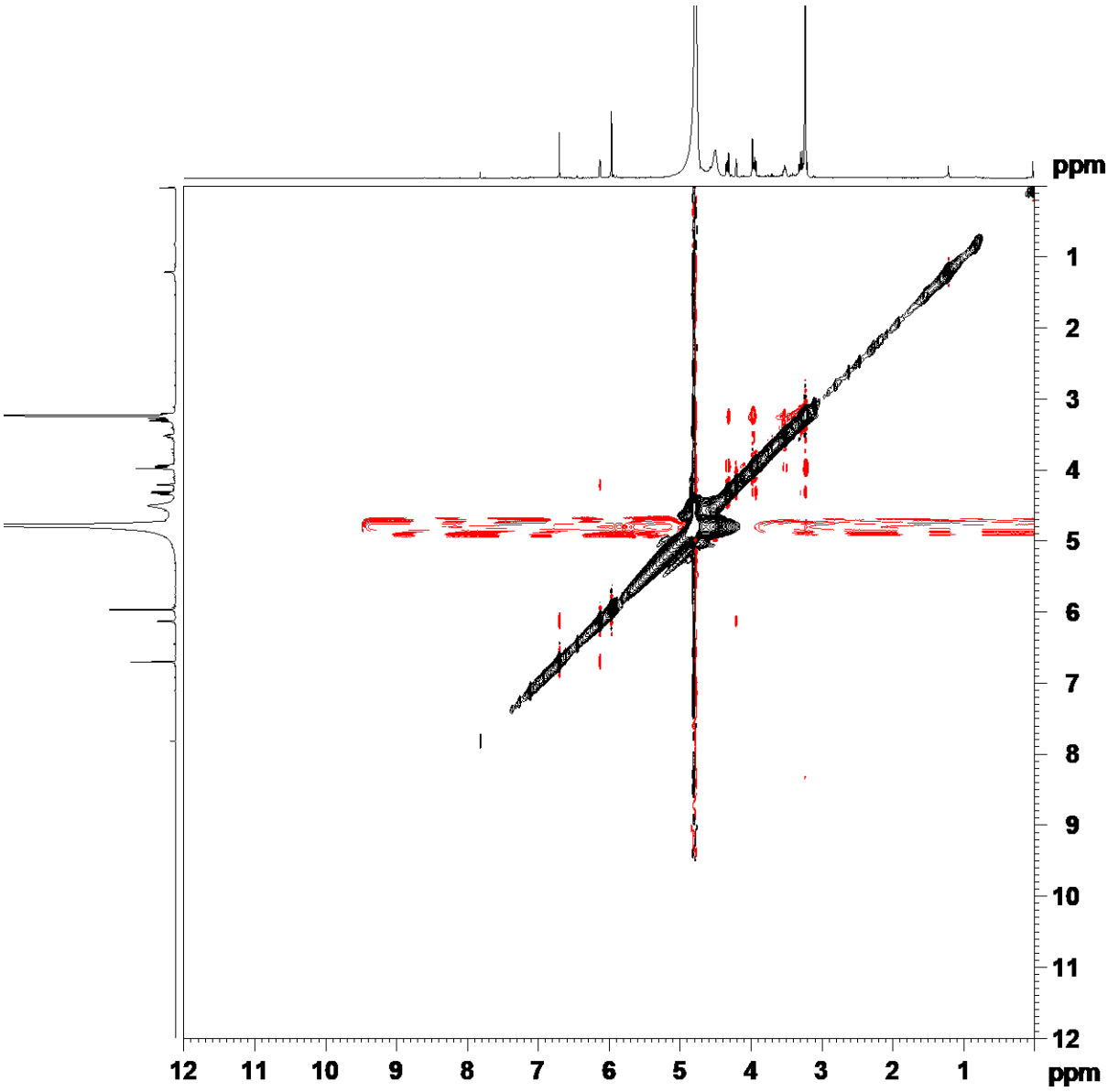

Figure S17. ^{1}H-^{1}H NOESY spectrum for compound 1 in MeOD-d_4

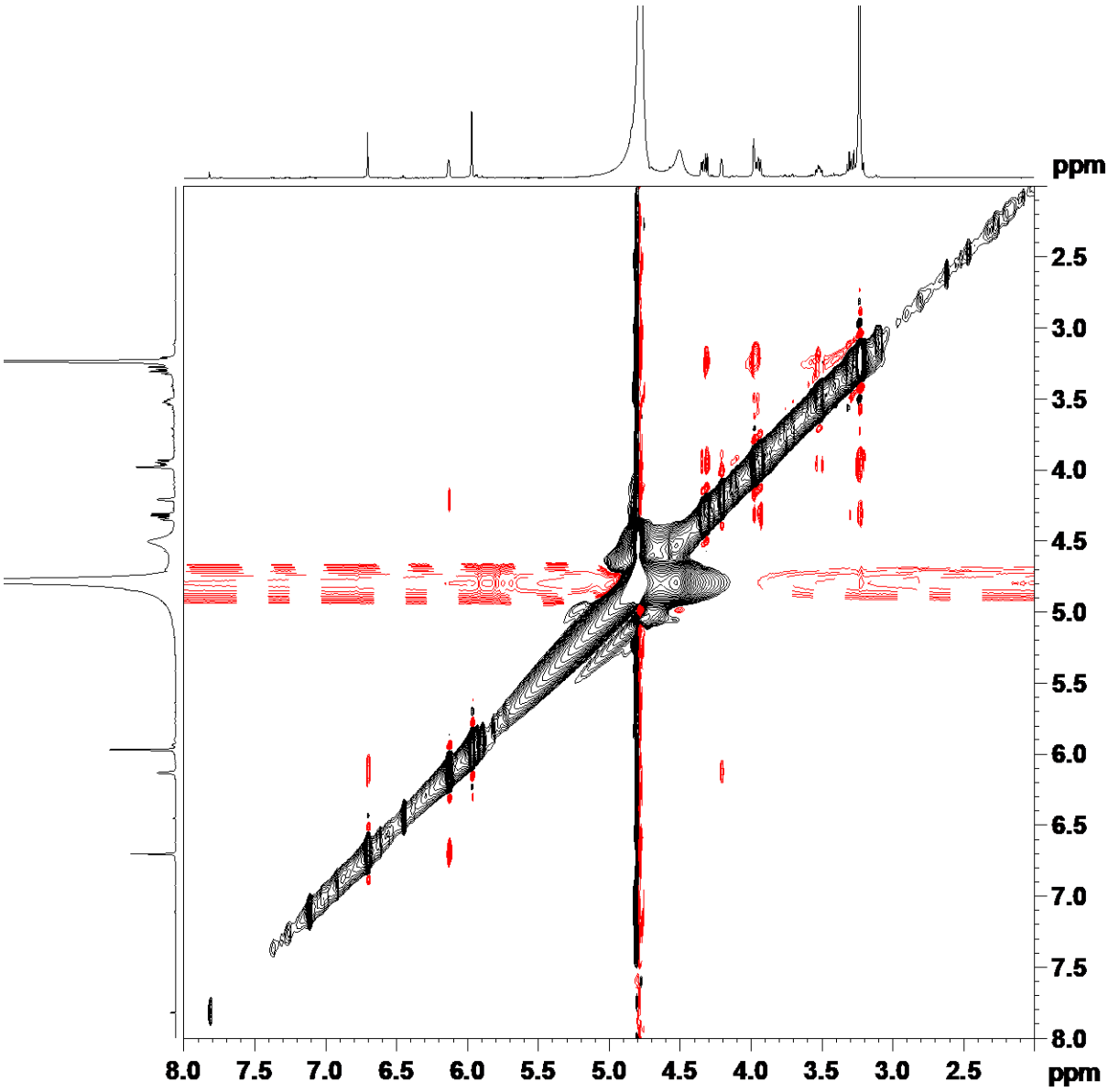

Figure S18. Expansion for ^{1}H-^{1}H NOESY spectrum for compound 1