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Supporting Information

for

Isolation and structure determination of a new analog of polycavernosides from marine *Okeania* sp. cyanobacterium

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NMR data for polycavernoside E (1)

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Table S1: Comparison of the carbon chemical shifts between polycavernosides E (**1**) and D (**5**) in $CDCl_3$.

position[1]	polycavernoside E (**1**)[2]	polycavernoside D (**5**)[3]
1	171.9, C	171.5, C
2	35.6, CH_2	35.5, CH_2
3	82.0, CH	81.9, CH
4	38.3, C	38.2, C
5[4]	85.3, CH	75.1, CH
6	37.7, CH_2	37.5, CH_2
7	83.8, CH	85.1, CH
8	42.1, CH_2	42.0, CH_2
9	206.9, C	206.5, C
10	103.0, C	102.6, C
11	39.7, CH	39.5, CH
12	33.6, CH_2	33.5, CH_2
13	83.5, CH	83.3, CH
14	39.8, C	39.7, C
15	78.4, CH	78.3, CH
16	127.4, CH	126.9, CH
17	135.4, CH	135.5, CH
18	130.1, CH	129.6, CH
19	133.9, CH	134.2, CH
20	131.2, CH	130.2, CH
21	134.6, CH	136.2, CH
27	13.3, CH_3	13.7, CH_3
28	17.8, CH_3	17.6, CH_3
29	19.4, CH_3	19.2, CH_3
30	22.2, CH_3	22.0, CH_3
31	13.9, CH_3	13.7, CH_3
1’	106.1, CH	106.0, CH
2’	83.8, CH	83.7, CH
3’	79.9, CH	79.9, CH
4’	78.5, CH	78.4, CH
5’	63.2, CH_2	63.1, CH_2
6’	61.1, CH_3	60.9, CH_3
7’	58.8, CH_3	58.6, CH_3
1”	103.0, CH	102.9, CH
2”	71.7, CH	71.6, CH
3”	71.0, CH	71.0, CH
4”	78.7, CH	78.7, CH
5”	60.1, CH_2	60.0, CH_2
6”	58.1, CH_3	58.0, CH_3

[1] The data from C-22 to C-26 were not included as they were useless for the discussion the relative configuration.

[2] Measured at 100 MHz.

[3] Measured at 151 MHz. Navarro, G.; Cummings, M. E.; Lee, J.; Moss, N.; Glukhov, E.; Valeriote, F. A.; Gerwick, L.; Gerwick, W. H. *Environ. Sci. Technol. Lett.* **2015**, *2*, 166-170.

[4] The chemical shift difference was big possibly due to the misassignment of the C-5 carbon chemical shift of **5**.

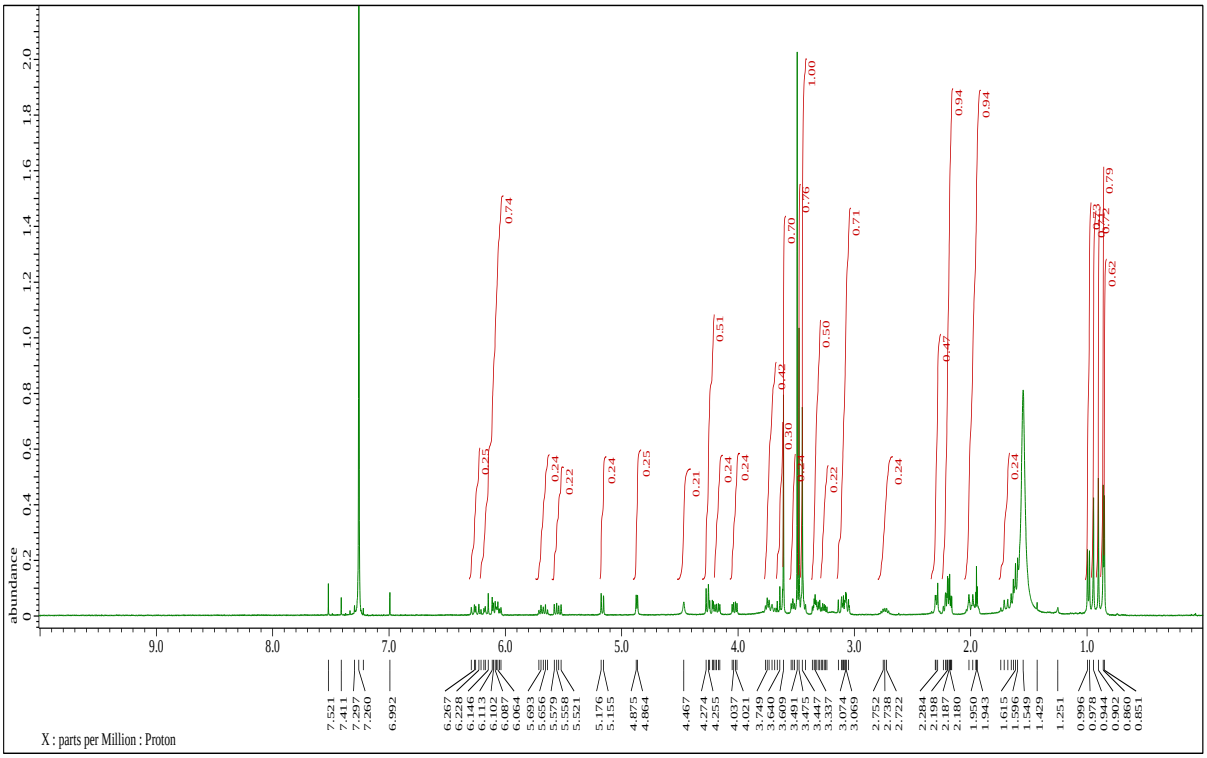
Table S2: Comparison of the proton chemical shifts of disaccharide moiety between **1** and **5** in $CDCl_3$.

position	polycavernoside E (**1**)[1]	polycavernoside D (**5**)[2]
1'	4.27, CH	4.27, CH
2'	3.07, CH_2	3.08, CH_2
3'	3.64, CH	3.64, CH
4'	3.27, CH	3.27, CH
5a'	4.03, CH_2	4.03, CH_2
5b'	3.12	3.12
6'	3.61, CH_3	3.61, CH_3
7'	3.45, CH_3	3.45, CH_3
1"	4.87, CH	4.86, CH
2"	3.53, CH	3.52, CH
3"	3.75, CH	3.74, CH
4"	3.34, CH	3.35, CH
5a"	4.23, CH_2	4.23, CH_2
5b"	3.46	3.46
6"	3.48, CH_3	3.48, CH_3

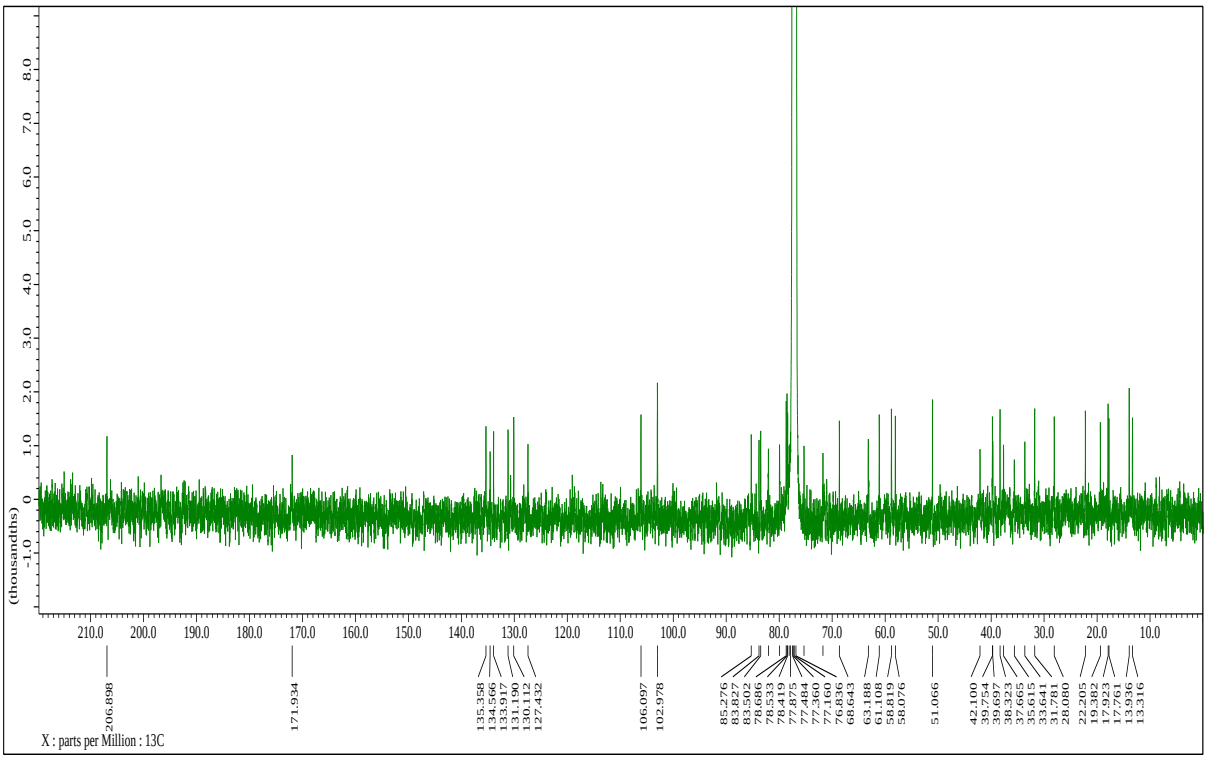
[1] Measured at 400 MHz.

[2] Measured at 600 MHz. Navarro, G.; Cummings, M. E.; Lee, J.; Moss, N.; Glukhov, E.; Valeriote, F. A.; Gerwick, L.; Gerwick, W. H. *Environ. Sci. Technol. Lett.* **2015**, *2*, 166-170.

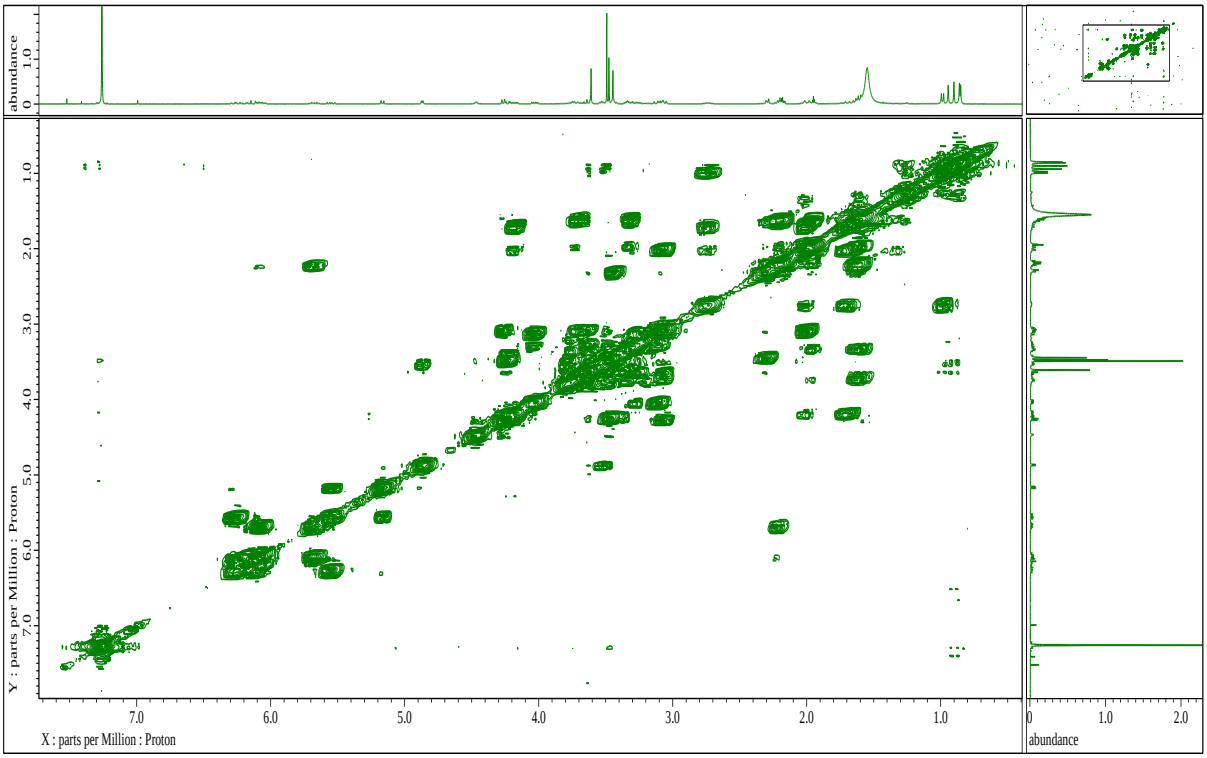
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of polycavernoside E (**1**)



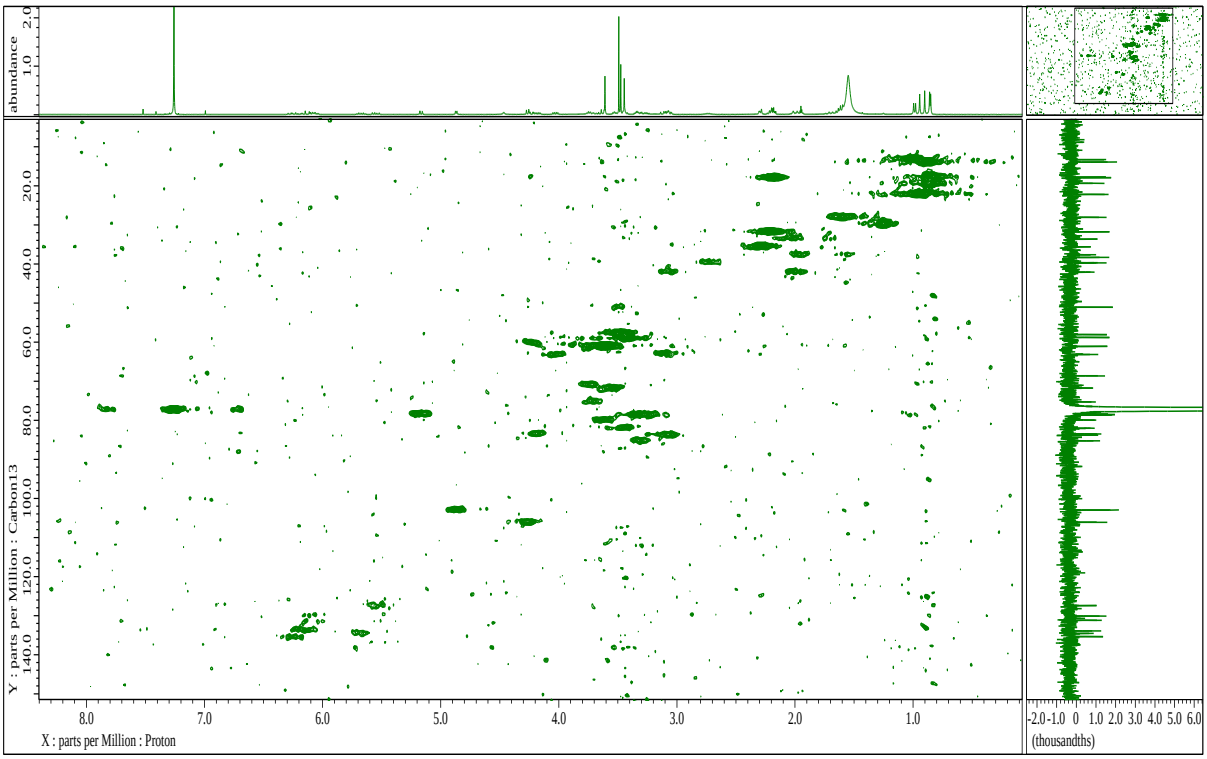
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of polycavernoside E (**1**)



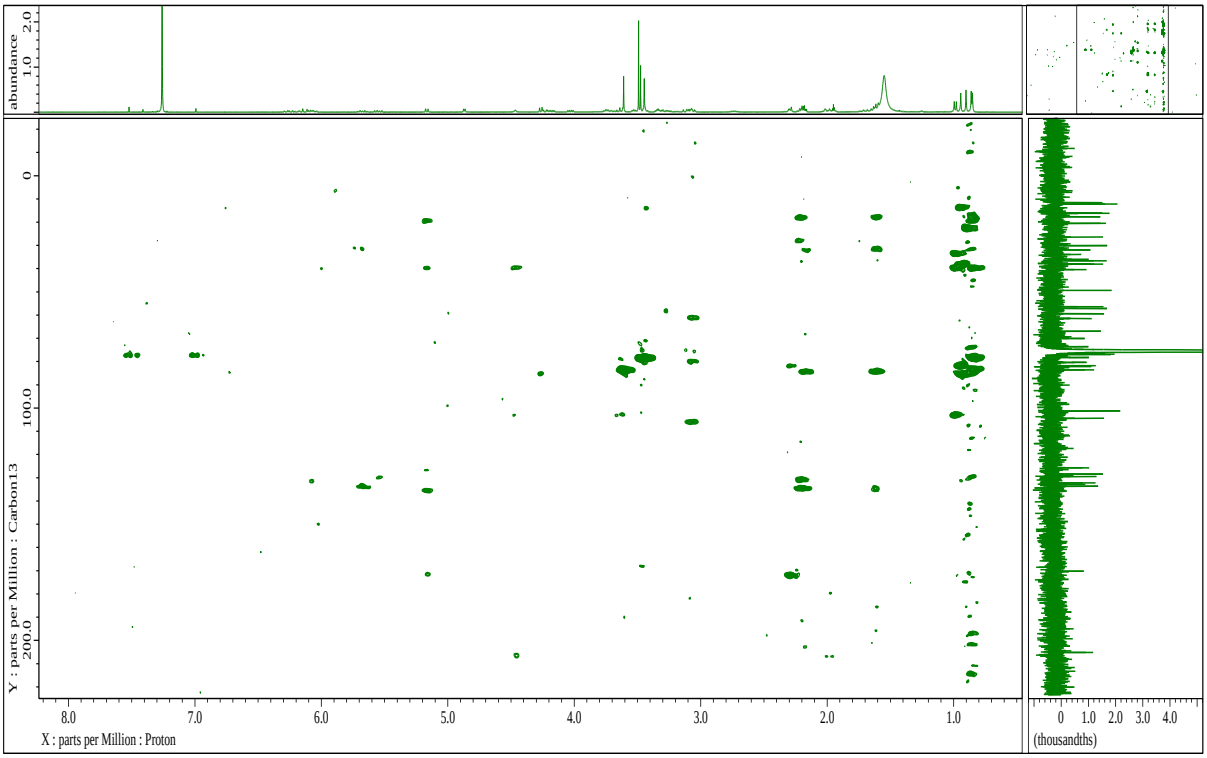
COSY (400 MHz, $CDCl_3$) spectrum of polycavernoside E (**1**)



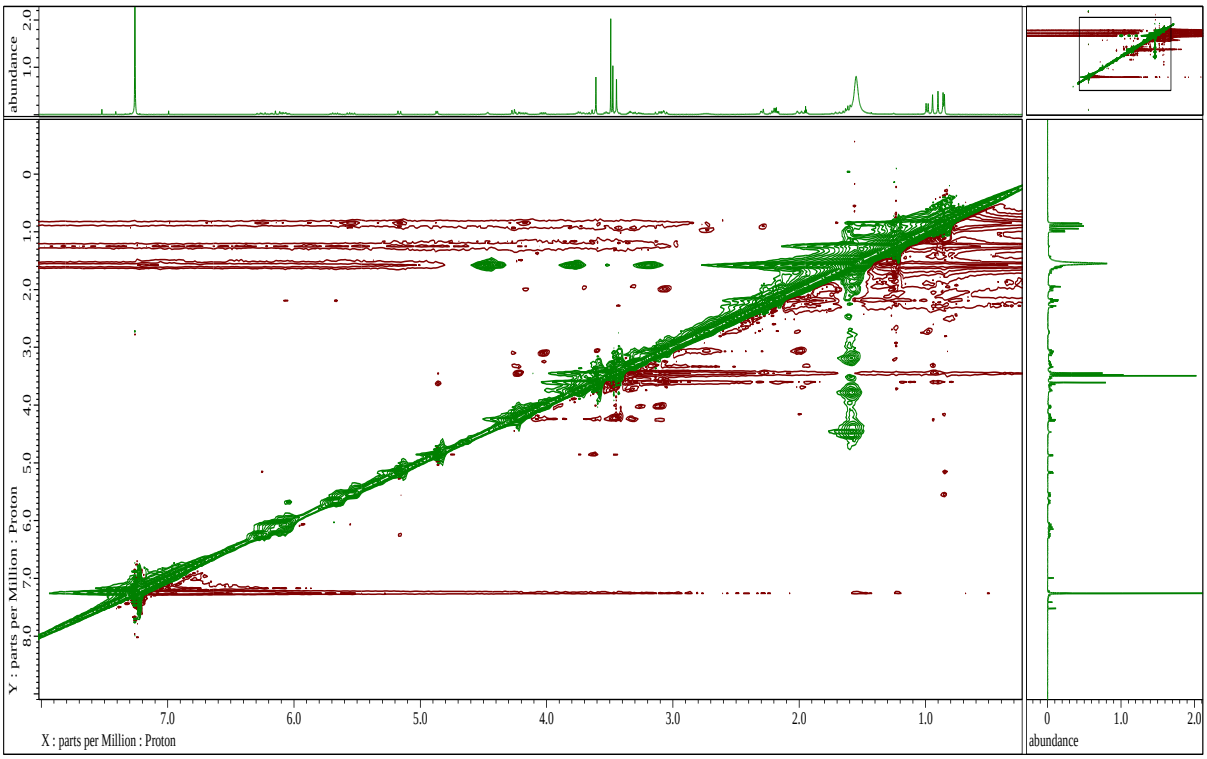
HMQC (400 MHz, $CDCl_3$) spectrum of polycavernoside E (**1**)



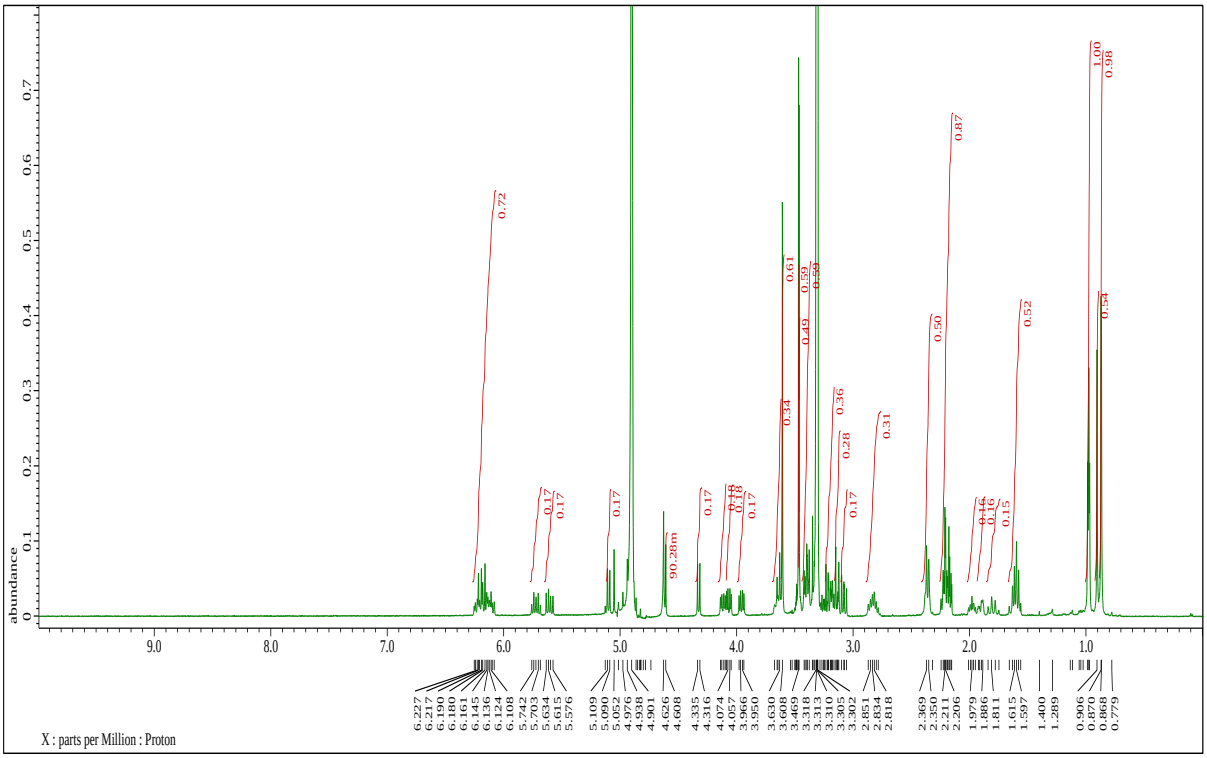
HMBC (400 MHz, $CDCl_3$) spectrum of polycavernoside E (**1**)



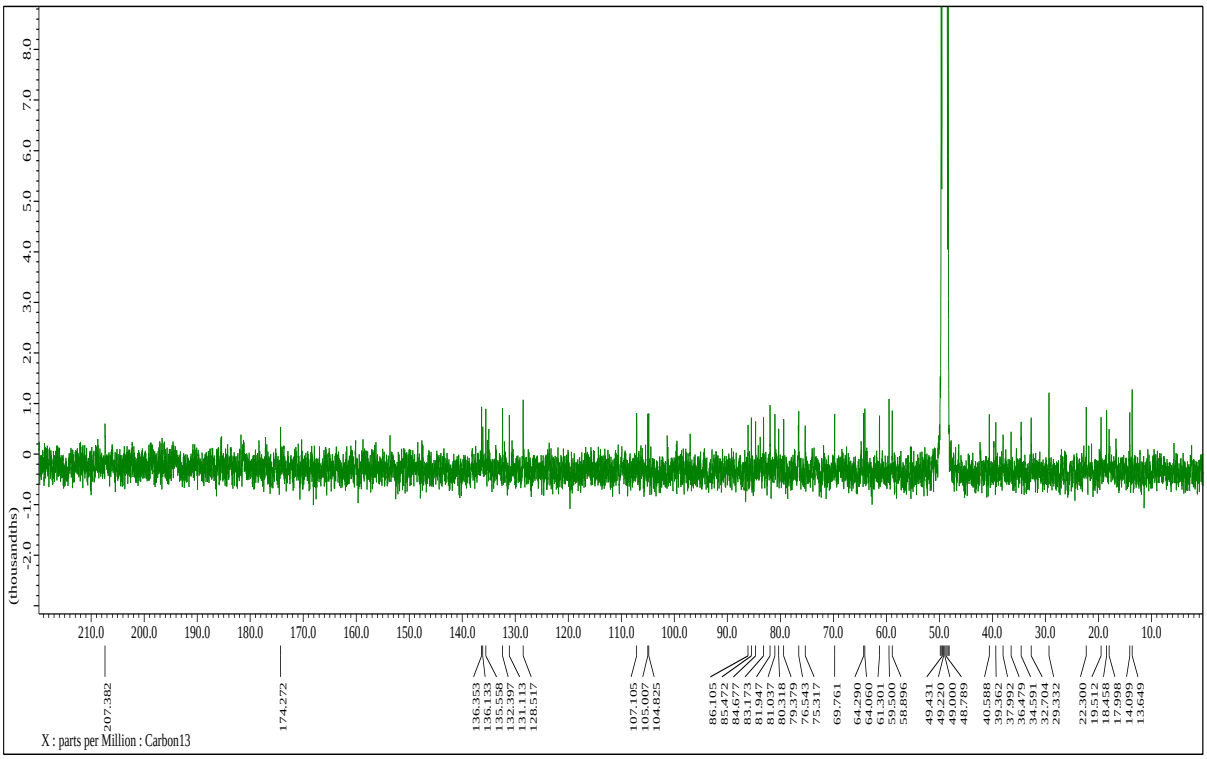
NOESY (400 MHz, $CDCl_3$) spectrum of polycavernoside E (**1**)



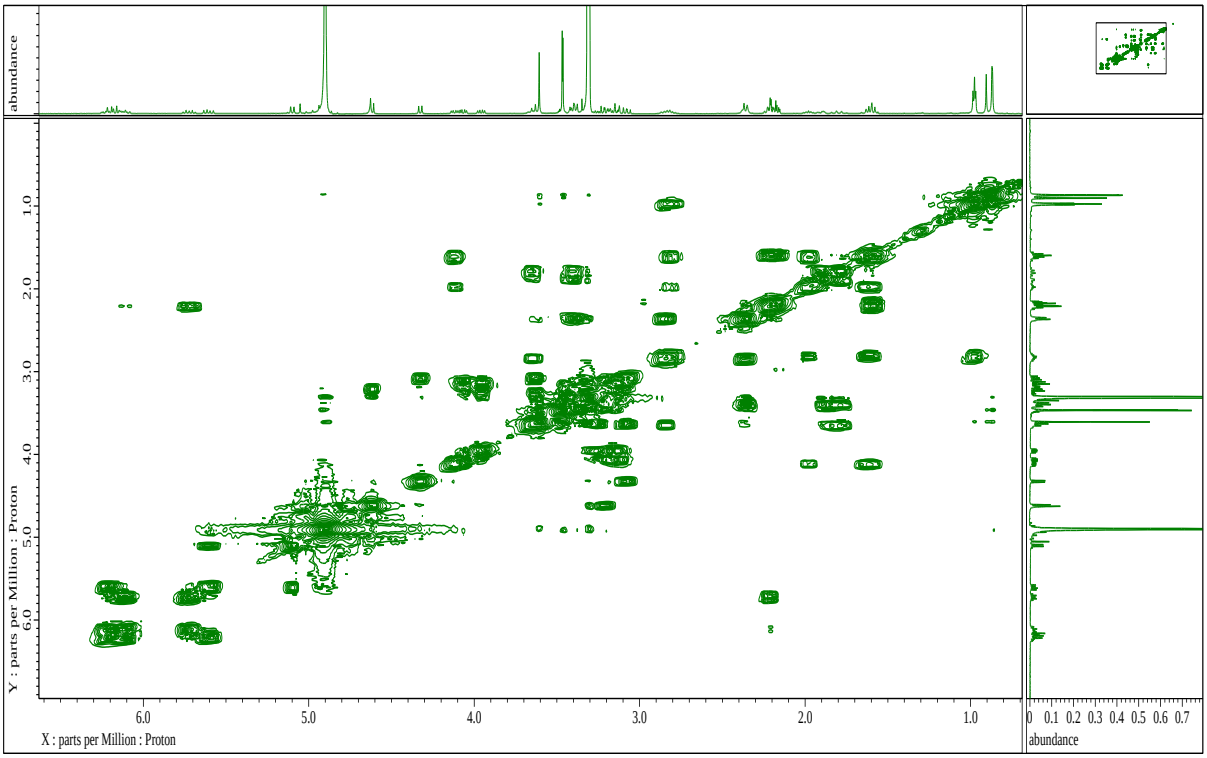
^{1}H NMR (400 MHz, CD_3OD) spectrum of polycavernoside E (**1**)



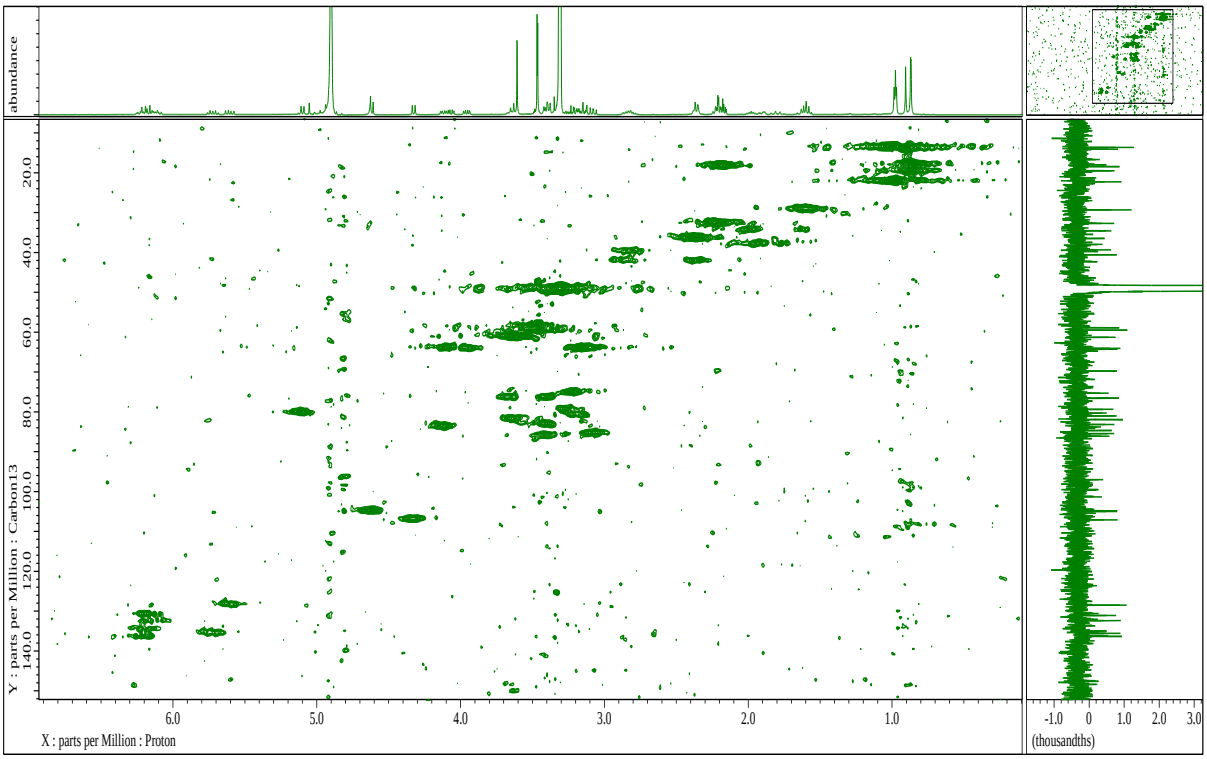
^{13}C{^{1}H} NMR (100 MHz, CD_3OD) spectrum of polycavernoside E (**1**)



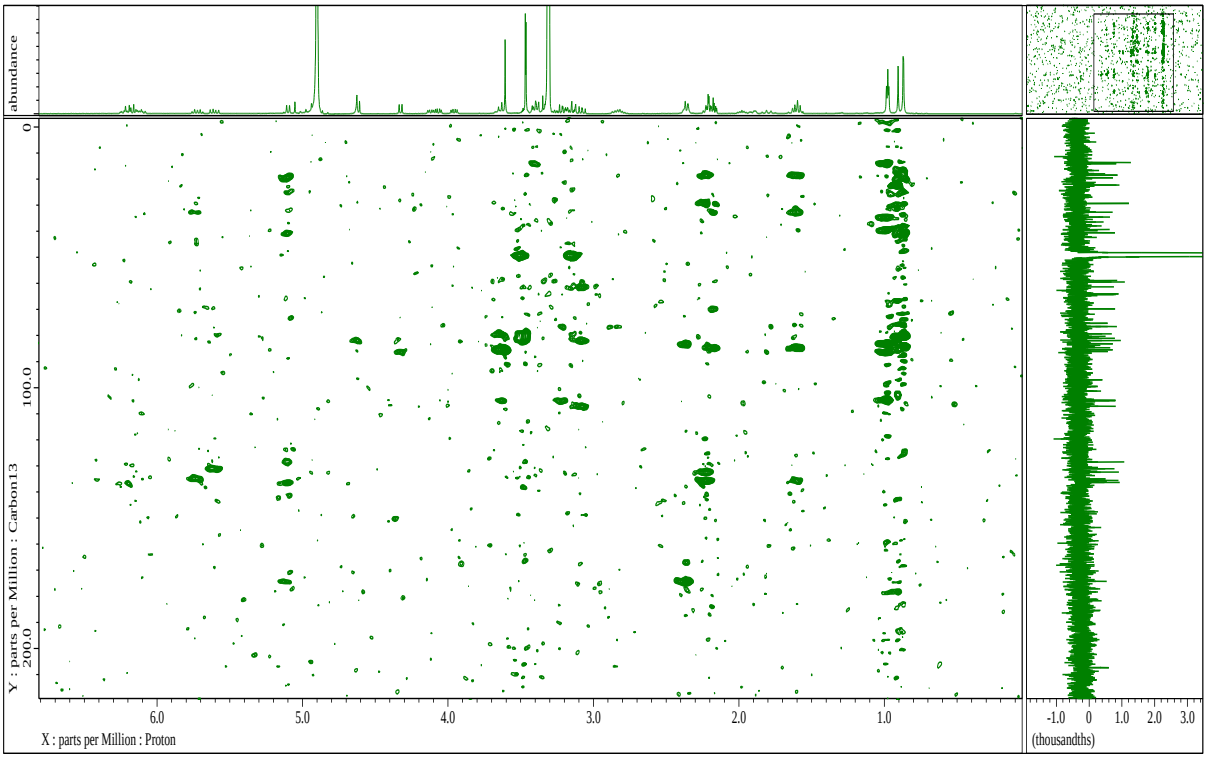
COSY (400 MHz, CD_3OD) spectrum of polycavernoside E (**1**)



HMQC (400 MHz, CD_3OD) spectrum of polycavernoside E (**1**)



HMBC (400 MHz, CD_3OD) spectrum of polycavernoside E (**1**)



NOESY (400 MHz, CD_3OD) spectrum of polycavernoside E (**1**)