Table S1 Sample information of CD1–CD13.

No.	Habitat	Part[#]	Processing[*]
1-GU-a	Alashan, Inner Mongolia	AP	a
1-GU-b	Alashan, Inner Mongolia	AP	b
1-GU-c	Alashan, Inner Mongolia	AP	c
1-GD-a	Alashan, Inner Mongolia	GP	a
2-GU-a	Alashan, Inner Mongolia	AP	a
2-GD-a	Alashan, Inner Mongolia	GP	a
3-GU-a	Alashan, Inner Mongolia	AP	a
3-GD-a	Alashan, Inner Mongolia	GP	a
4-GU-a	Yongning, Ningxia	AP	a
4-GU-b	Yongning, Ningxia	AP	b
4-GU-c	Yongning, Ningxia	AP	b
4-GD-a	Yongning, Ningxia	GP	a
4-GD-b	Yongning, Ningxia	GP	b
4-GD-c	Yongning, Ningxia	GP	c
5-GU-a	Yongning, Ningxia	AP	a
5-GD-a	Yongning, Ningxia	GP	a
6-GU-a	Yongning, Ningxia	AP	a
6-GD-a	Yongning, Ningxia	GP	a
7-GU-a	Yongning, Ningxia	AP	a
7-GD-a	Yongning, Ningxia	GP	a
8-GU-a	Yongning, Ningxia	AP	a
8-GD-a	Yongning, Ningxia	GP	a
9-GU-a	Tamusu, Alashan, Inner Mongolia	AP	a
9-GD-a	amusu, Alashan, Inner Mongolia	GP	a
10-GD-a	Suhaitugacha, Alashan, Inner Mongolia	GP	a
10-GD-b	Suhaitugacha, Alashan, Inner Mongolia	GP	b
10-GD-c	Suhaitugacha, Alashan, Inner Mongolia	GP	c
11-GU-a	Suhaitugacha, Alashan, Neimenggu	AP	a
11-GD-a	Suhaitugacha, Alashan, Neimenggu	GP	a
12-G-a	Tazhong, Xinjiang	WP	a
12-G-b	Tazhong, Xinjiang	WP	b
12-G-c	Tazhong, Xinjiang	WP	c

[#]: AP, the upper parts; GP, the lower parts; WP, the whole plant;

*: a, successively steamed for 10 min and oven-dried at 60 °C for 48 h; b, direct freeze-drying; c, freeze-drying hyphenated with sequential 10 min-steaming.

Table S2 Signal assignment of the ^{1}H NMR spectrum of CD

No.	Compound	Proton signal assignment
1	Nicotinamide	9.15 (br s), 8.88, 8.09
2	Formic acid	8.48 (s)
3	Adenosine	8.14, 8.12
4	Adenine	8.13, 8.10
5	Cistanoside B/D	7.73 (d, *J* =16.0 Hz)
6	Echinacoside*	7.60 (1H, d, *J* =16.0 Hz, H-7′), 6.28 (1H, d, *J* = 16.0 Hz, H-8′), 7.06 (1H, br s, Hz, H-2′), 6.96 (1H,br d, *J* = 8.0 Hz, H-6′), 6.78 (1H, d, *J* = 8.0 Hz, H-5′), 6.71 (1H, br s, H-2), 6.68 (1H, d, *J* = 8.0 Hz, H-5), 6.58 (1H, br d, *J* = 8.0 Hz, H-6), 2.80 (2H, m, H-7), 4.39 (1H, d, *J* = 8.0 Hz, H-1‴), 4.30 (1H, d, *J* = 7.5 Hz, H-1″), 5.18 (1H, br s, H-1‴), 1.09 (3H,d, *J* = 6.0 Hz, H-6‴)
7	Acteoside*	7.59 (1H, d, *J* = 16.0 Hz, H-7′), 6.28 (1H, d, *J* = 16.0 Hz, H-8′), 7.01 (1H,d, *J* = 1.5 Hz, H-2′), 6.96 (1H, dd, *J* = 1.5, 8.0 Hz, H-6′), 6.78 (1H, d, *J* = 8.0 Hz, H-5′), 6.70 (1H, d, *J* = 1.5 Hz, H-2), 6.68 (1H, d, *J* = 8.0 Hz, H-5), 6.57 (1H, dd, *J* =1.5, 8.0 Hz, H-6), 2.80-2.83 (2H, m, H-7), 4.38 (1H, d, *J* = 7.5 Hz, H-1″), 5.19 (1H,br s, H-1‴), 1.09 (3H, d, *J* = 5.5 Hz, H-6‴)
8	Isoacteoside	7.58 (d, *J* =16.0 Hz)
9	Indole 3-acetic acid	7.40 (d, *J* = 7.0 Hz)
10	Phenylalanine	7.33
11	Tyrosine	7.12
12	Syringaresinolor its glucoside	7.02
13	*cis*-type PhGs	6.95 (d, *J* =12.0 Hz)
14	Citrusin A/Alaschanioside A/Dehydeodiconiferyl Alcohol glucoside	6.56 – 6.64
15	Fumaric acid	6.54
16	Iridoids	6.18 – 6.33
17	Maleic acid	6.02
18	Sucrose*	5.41 (d, *J* = 3.6 Hz), 4.18 (d, *J* = 7.8 Hz), 4.04 (t, *J* = 7.8 Hz)

19	*β*-Galactose*	5.24 (d, *J* = 5.0 Hz)
20	*α*-Glucose*	5.20 (d, *J* = 3.7 Hz)
21	*β*-Glucose	4.60 (d, *J* = 7.8 Hz)
22	Malic acid	4.27 (dd, *J* = 2.8, 10.0 Hz), 2.67 (dd, *J* = 3.0, 15.5 Hz), 2.37 (dd, *J* = 10.0, 15.5 Hz)
23	Proline	4.09 (m)
24	Mannitol*	4.00 (d, *J* = 10.3 Hz)
25	Methoxyl group of phenyl derivatives	3.80 – 3.81
26	Isocitric acid	3.04
27	Asparagine acid	2.96
28	Citric acid	2.73
29	Ketoglutaric acid	2.52
30	Pyruvic acid	2.49
31	Succinic acid	2.42 (s)
32	Glutamine	2.30
33	Acetyl of phenyl derivatives	1.97 (s)
34	Lysine	1.71
35	Alanine	1.49 (d, *J* = 7.0 Hz)
36	Fatty acid	1.32 – 1.35 (m)
37	Threonine	1.27 (m)
38	1-*O*-ethyl-glucoside	1.16 (m)
39	Rha of sugars or PhGs	1.06 (d, *J* = 6.0 Hz)
40	8-Epiloganic acid	1.03 (d, *J* = 7.0 Hz)
41	Isoleucine/Valine	0.98
42	Leucine	0.93

Note: the components marked with * were identified with the assistance of reference compounds.

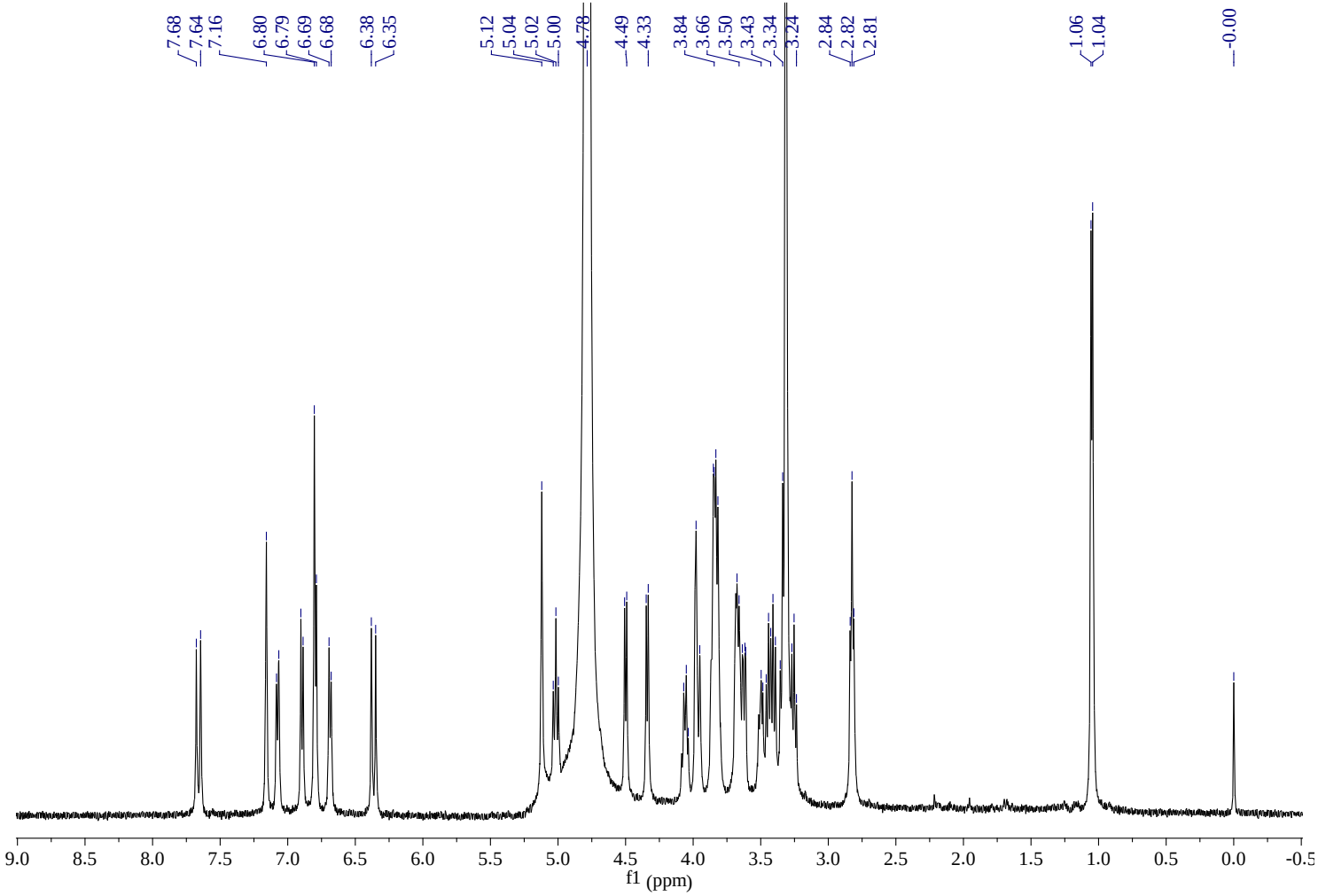

Figure S1 ^{1}H NMR spectrum of echinacoside (CD_3OD:D_2O=1:1, 500 MHz).

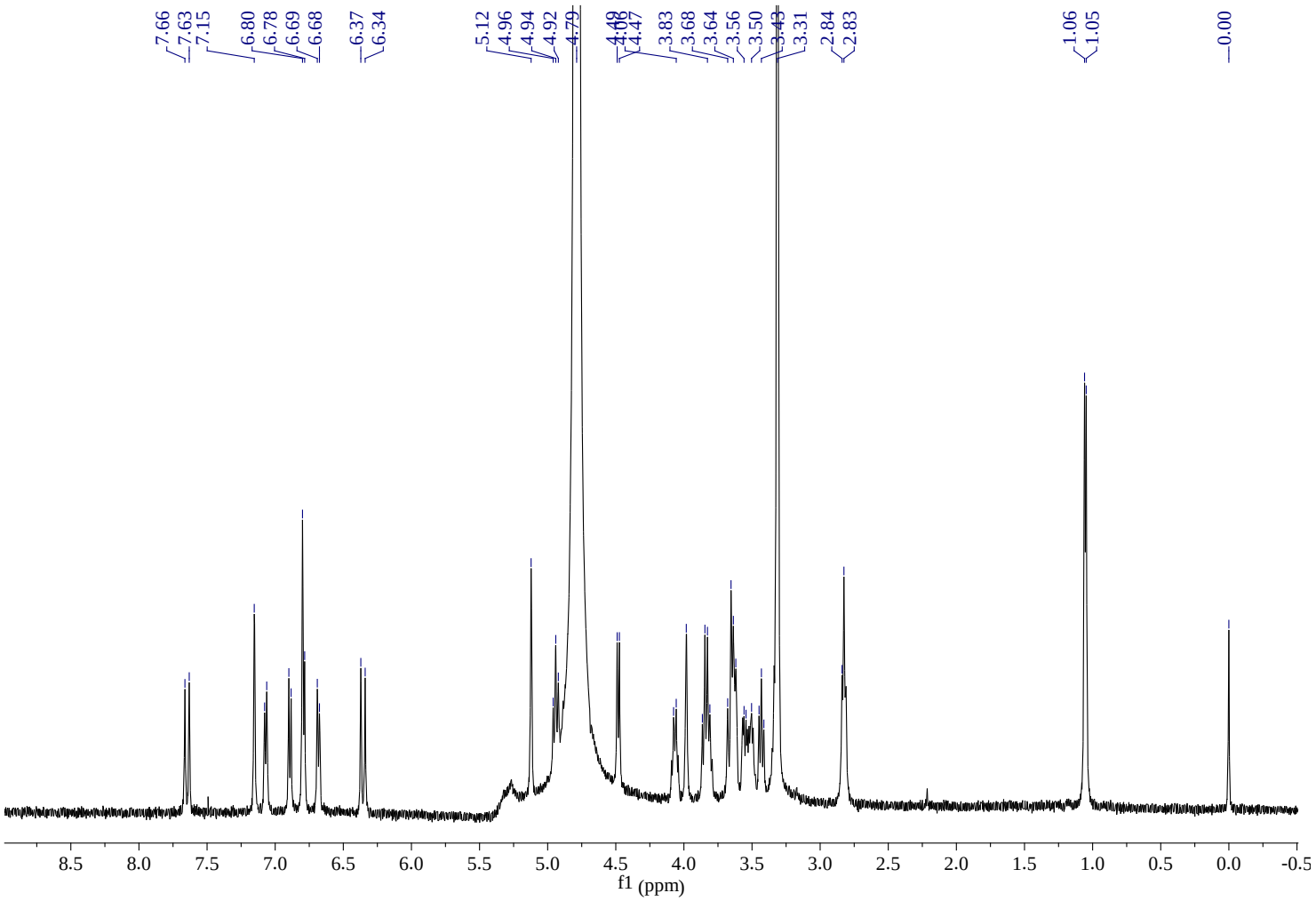

Figure S2 ^{1}H NMR spectrum of verbascoside (also known as acteoside) (CD_3OD:D_2O=1:1, 500 MHz).

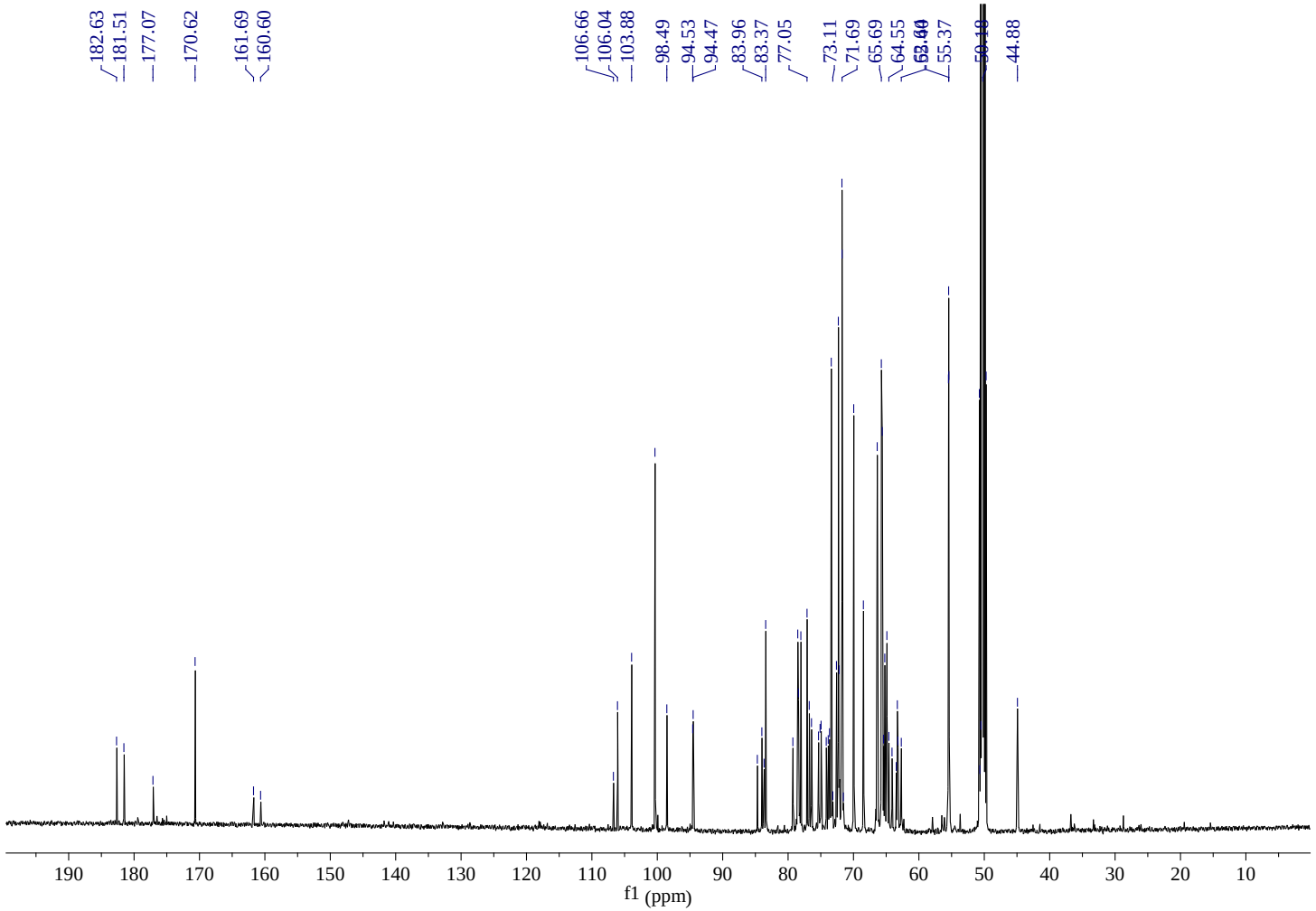

Figure S3 Representative ^{13}C NMR spectrum of *C. deserticola* (CD_3OD:D_2O=1:1, 500 MHz).

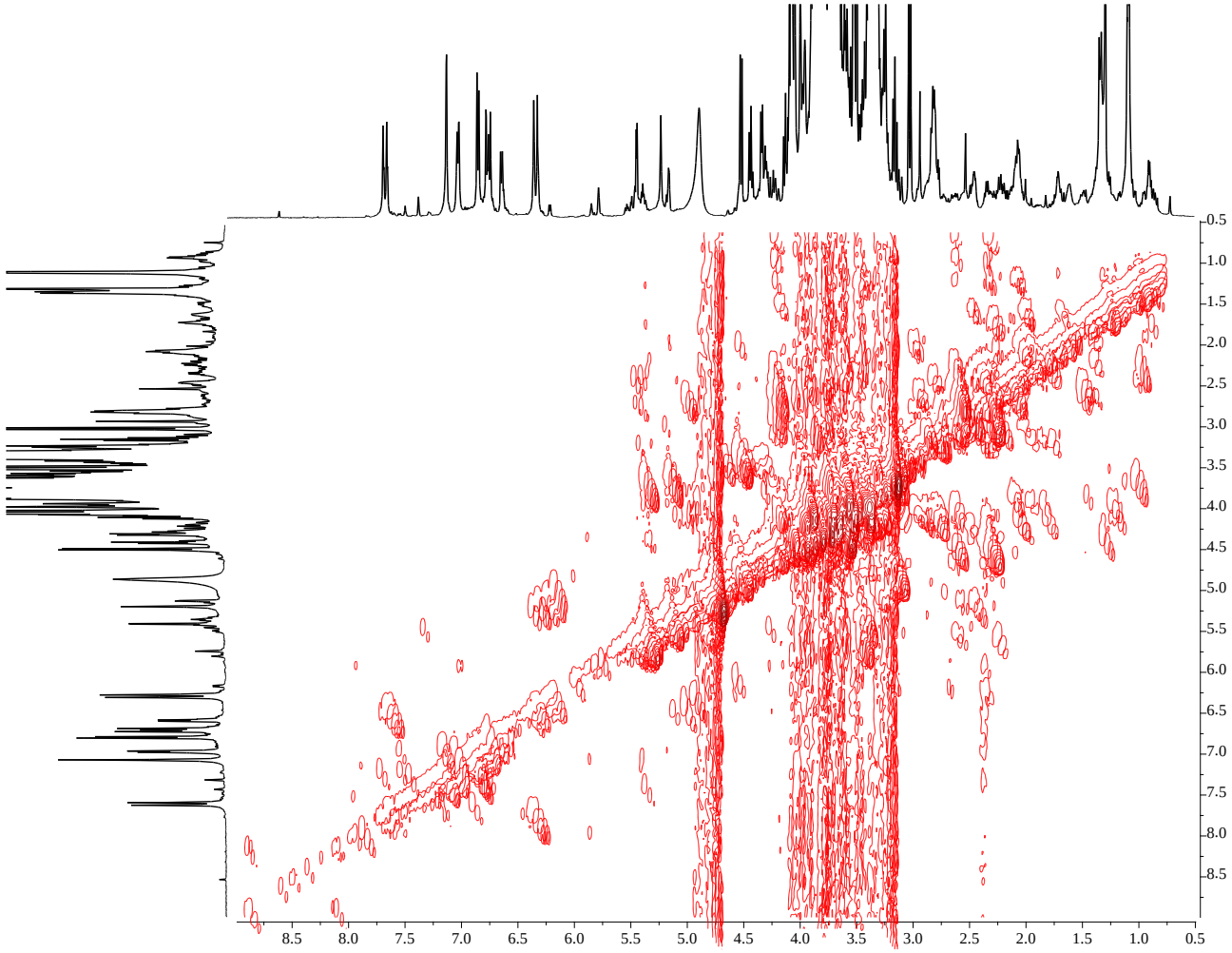

Figure S4 Representative $^{1}H–^{1}H$ COSY spectrum of *C. deserticola* ($CD_3OD:D_2O$=1:1, 500 MHz).

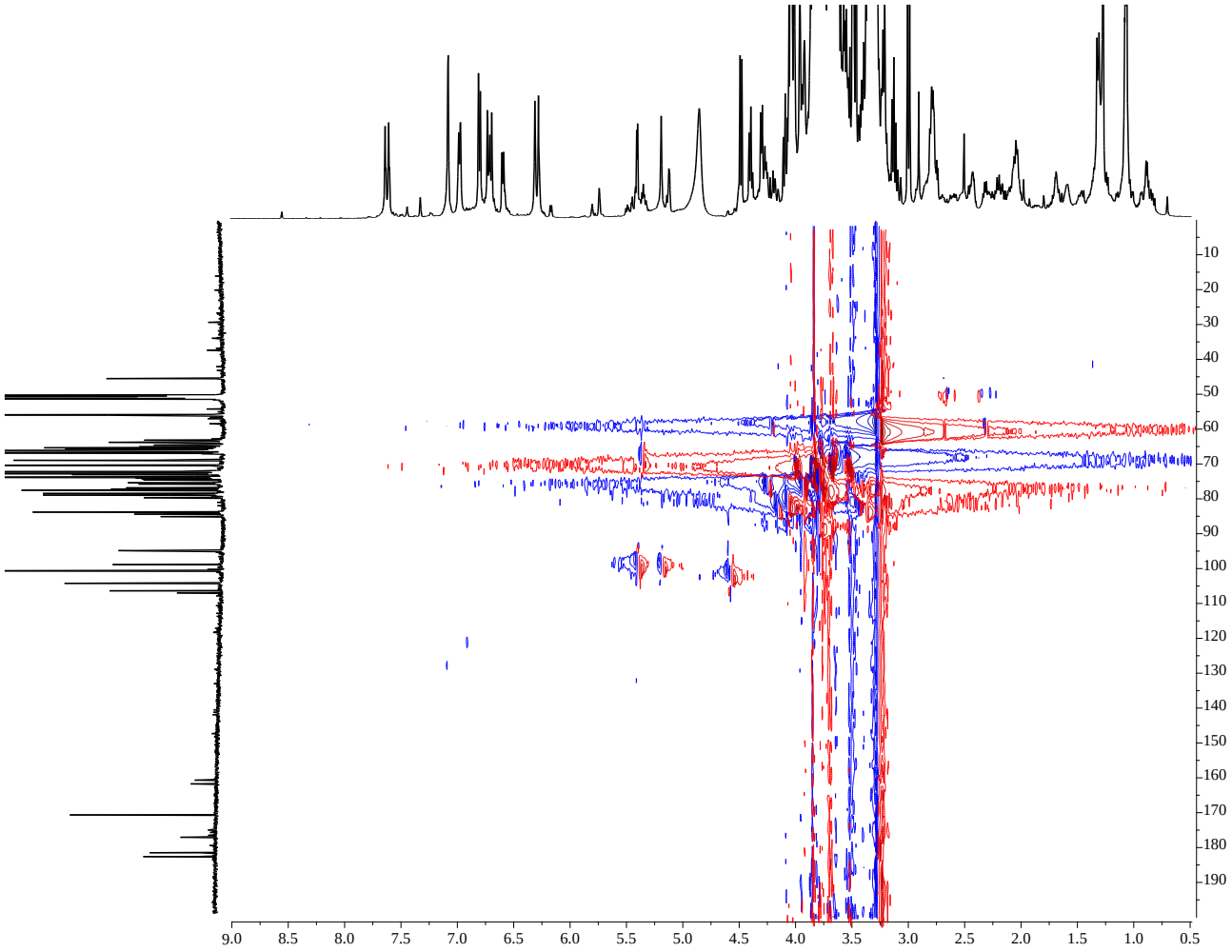

Figure S5 Representative HSQC spectrum of *C. deserticola* (CD_3OD:D_2O=1:1, 500 MHz).

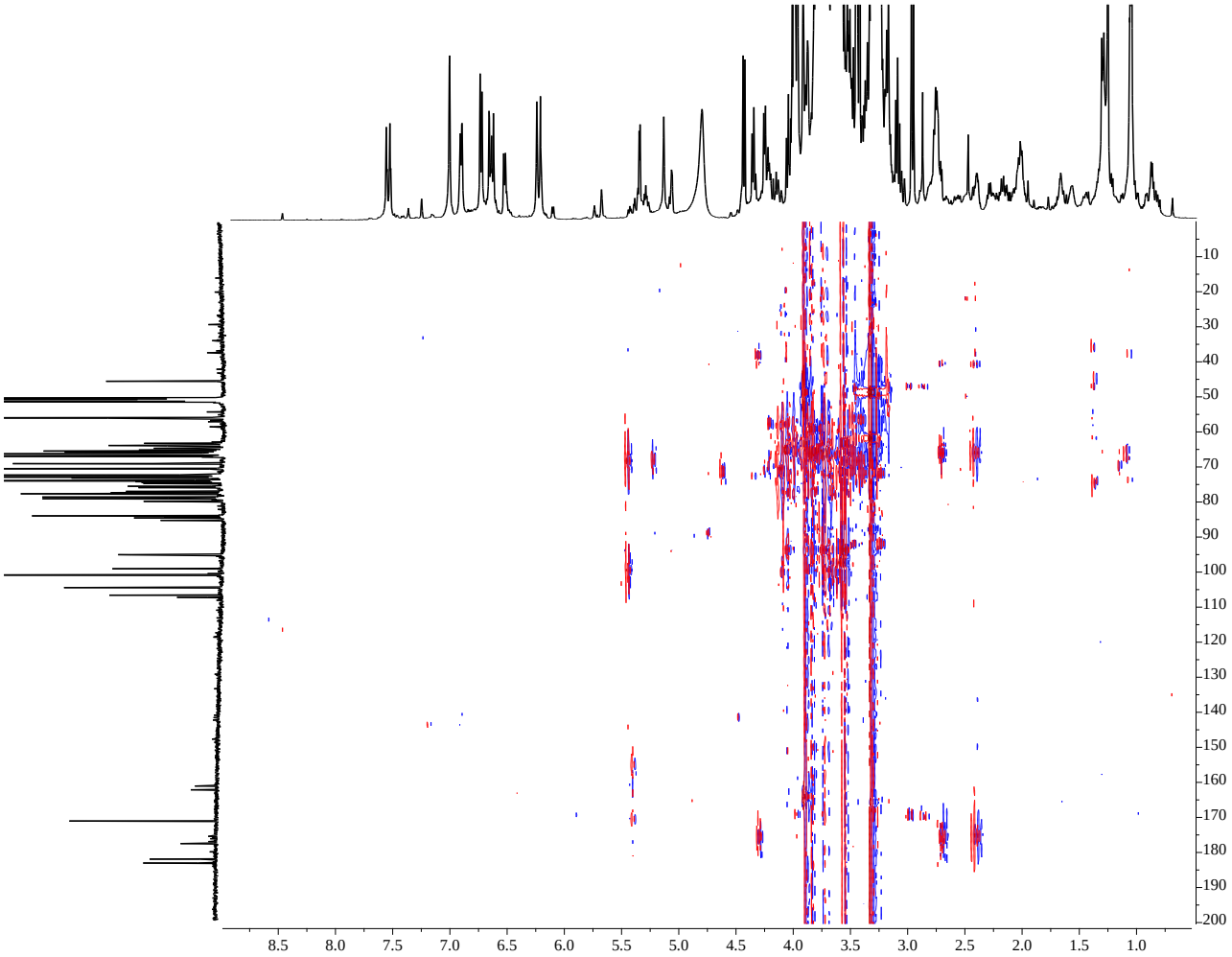

Figure S6 Representative HMBC spectrum of *C. deserticola* (CD_3OD:D_2O=1:1, 500 MHz).

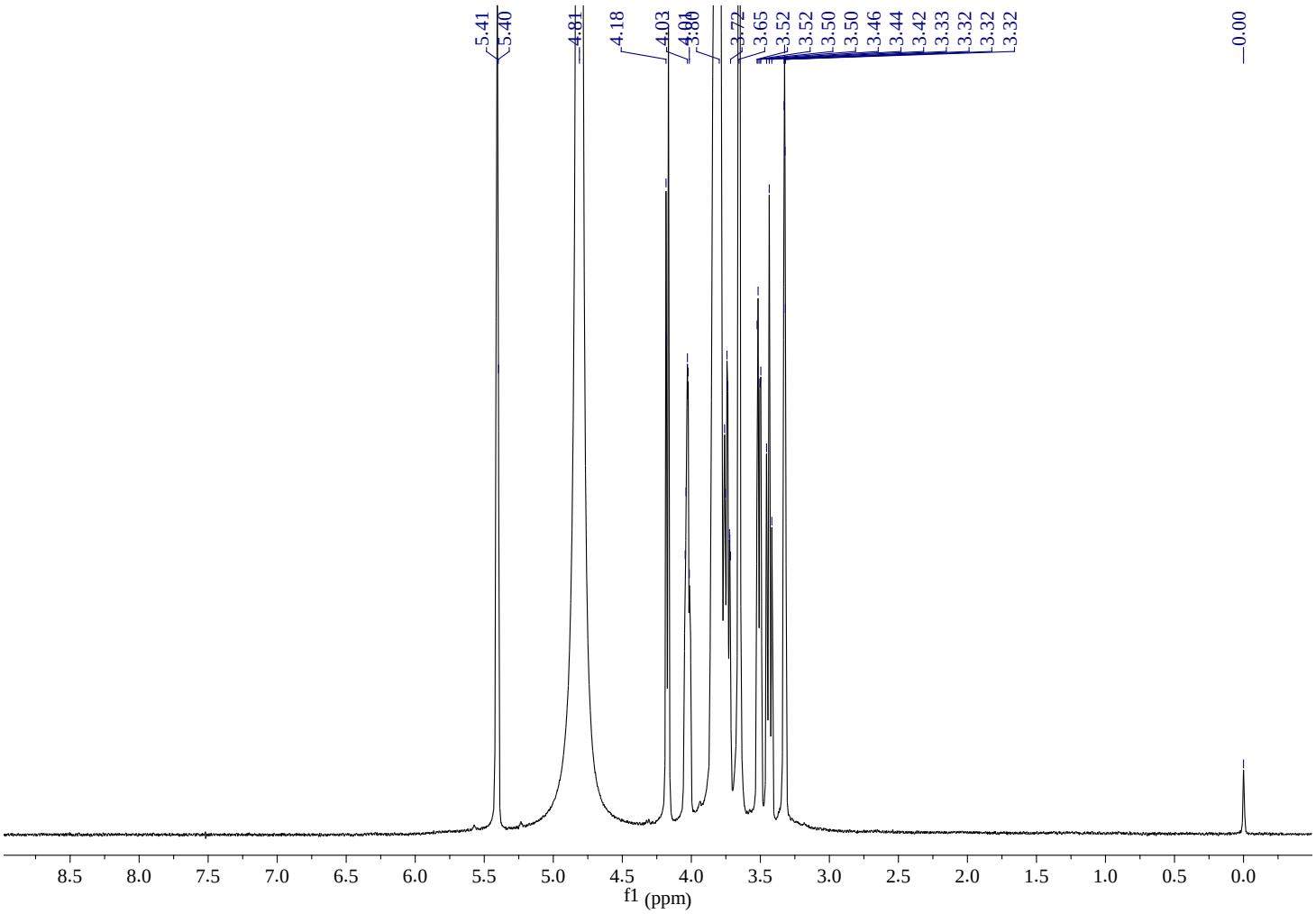

Figure S7 ^{1}H NMR spectrum of sucrose (CD_3OD:D_2O=1:1, 500 MHz).

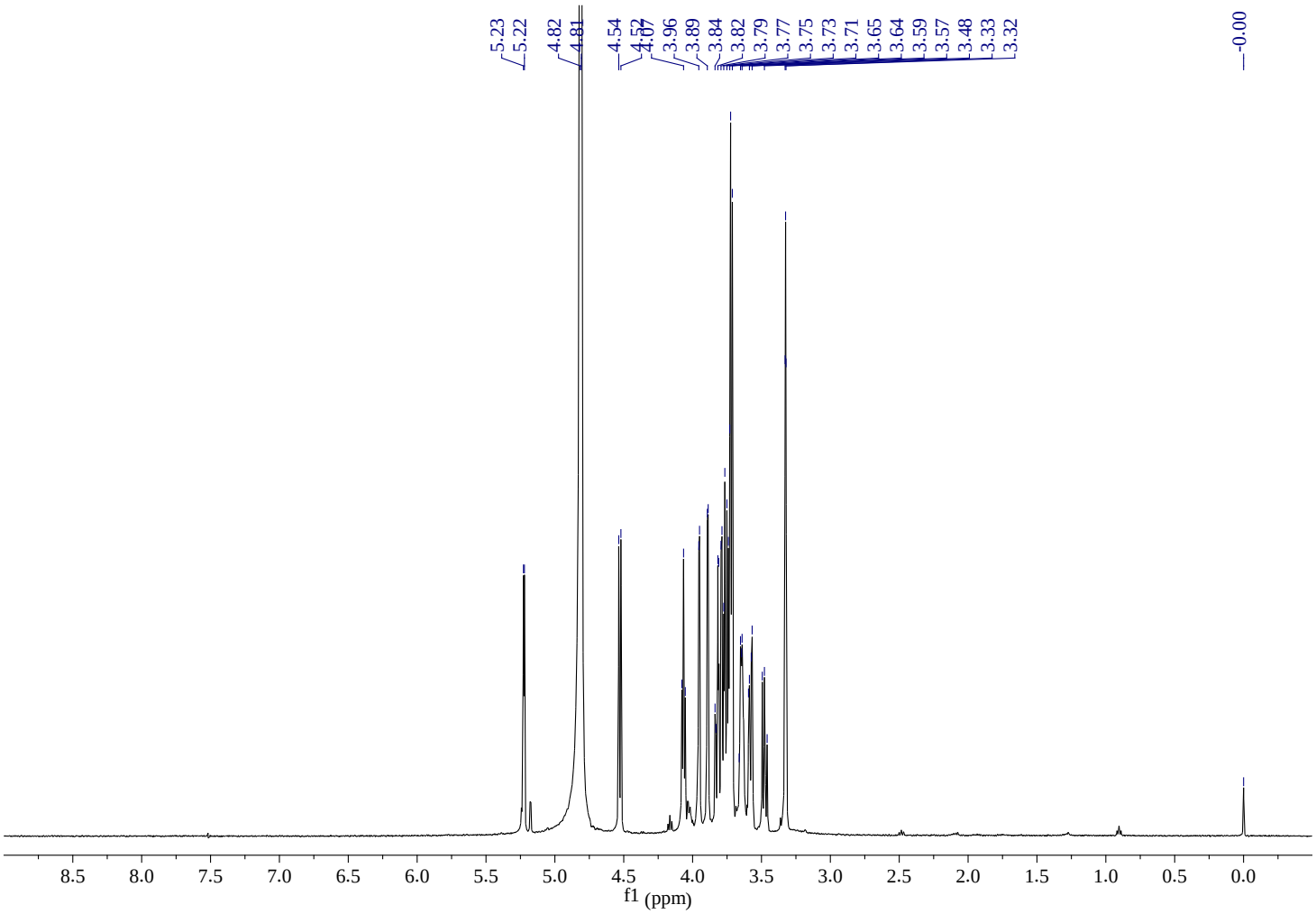

Figure S8 ^{1}H NMR spectrum of *β*-galactose (CD_3OD:D_2O=1:1, 500 MHz).

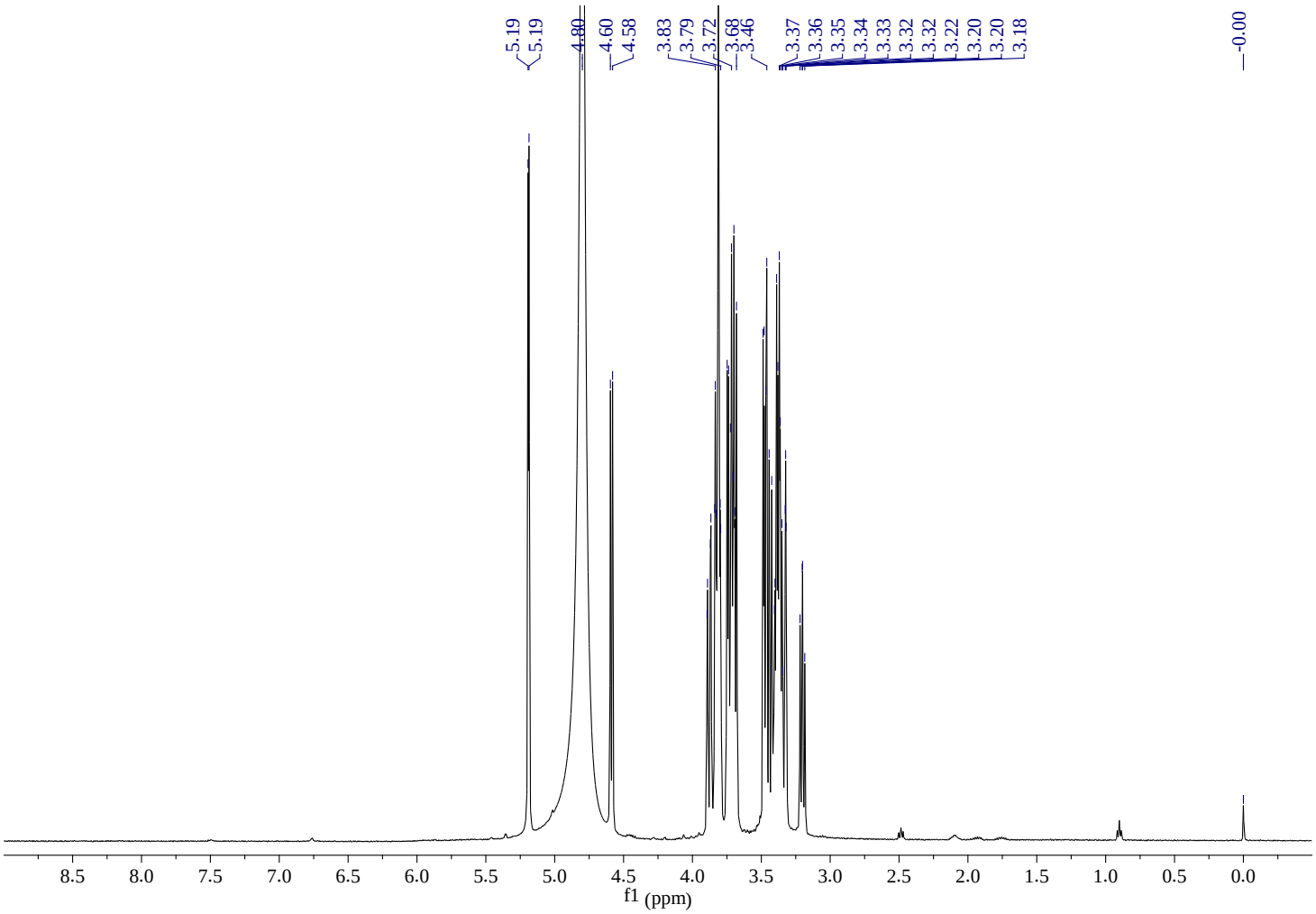

Figure S9 ^{1}H NMR spectrum of β-glucose (CD_3OD:D_2O=1:1, 500 MHz).

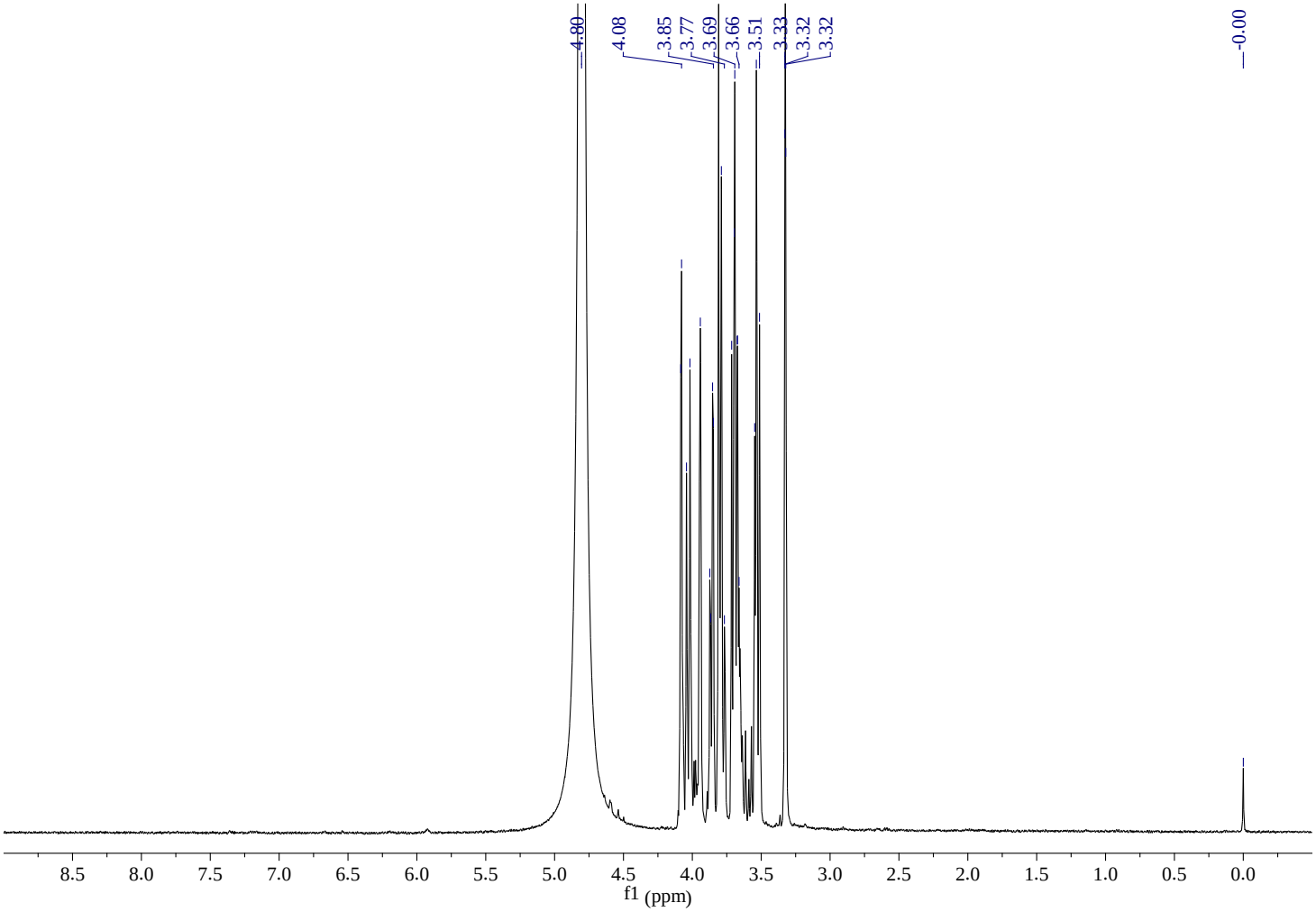

Figure S10 ^{1}H NMR spectrum of mannitol (CD_3OD:D_2O=1:1, 500 MHz).