Supporting information for:

A Simple Synthesis Route for Selectively Methylated *β*-cyclodextrin Using a Copper Complex Sandwich Protecting Strategy

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S1. NMR and MALDI-TOF Spectra

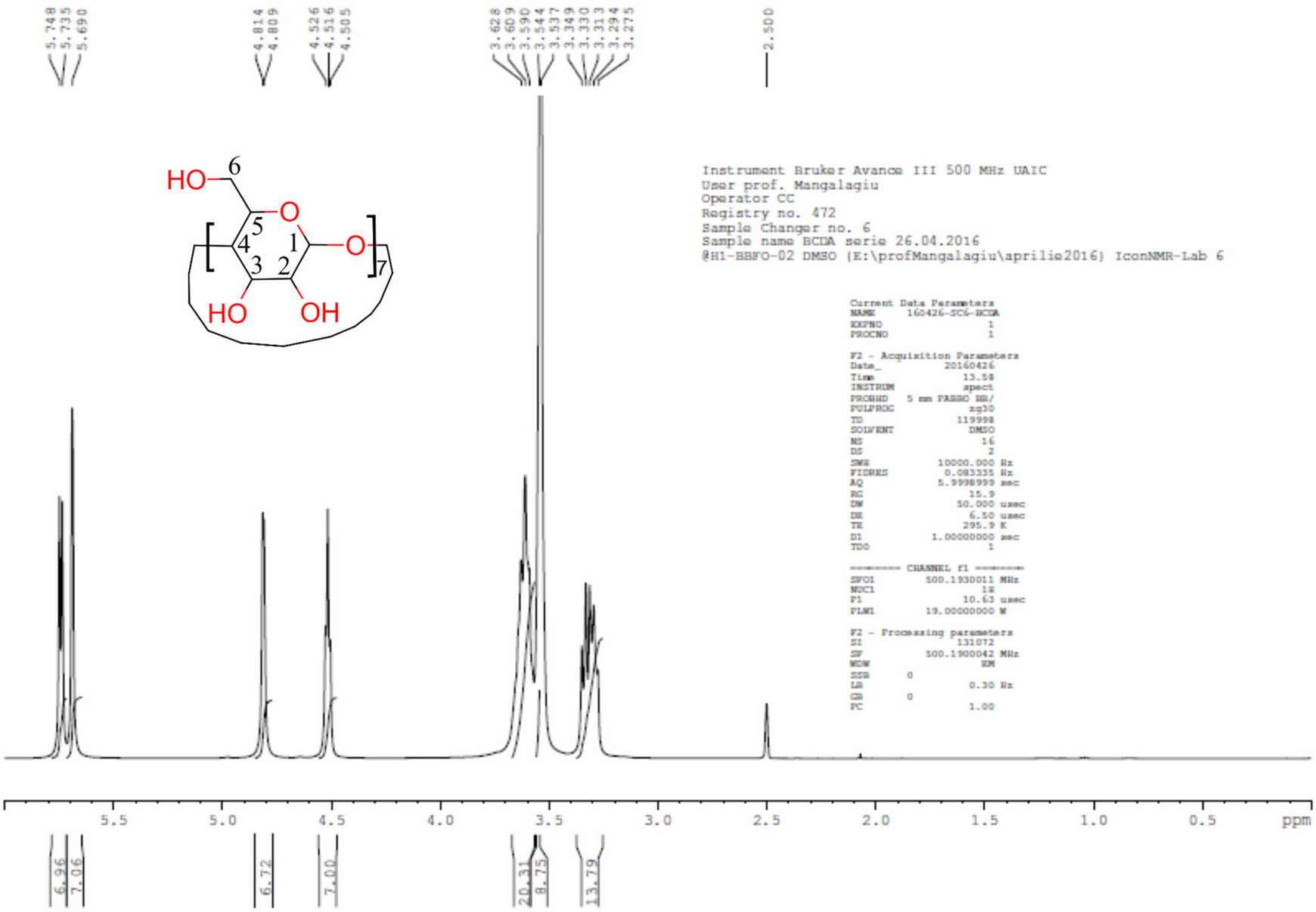

Figure S1. ^{1}H-NMR spectrum of β-CD

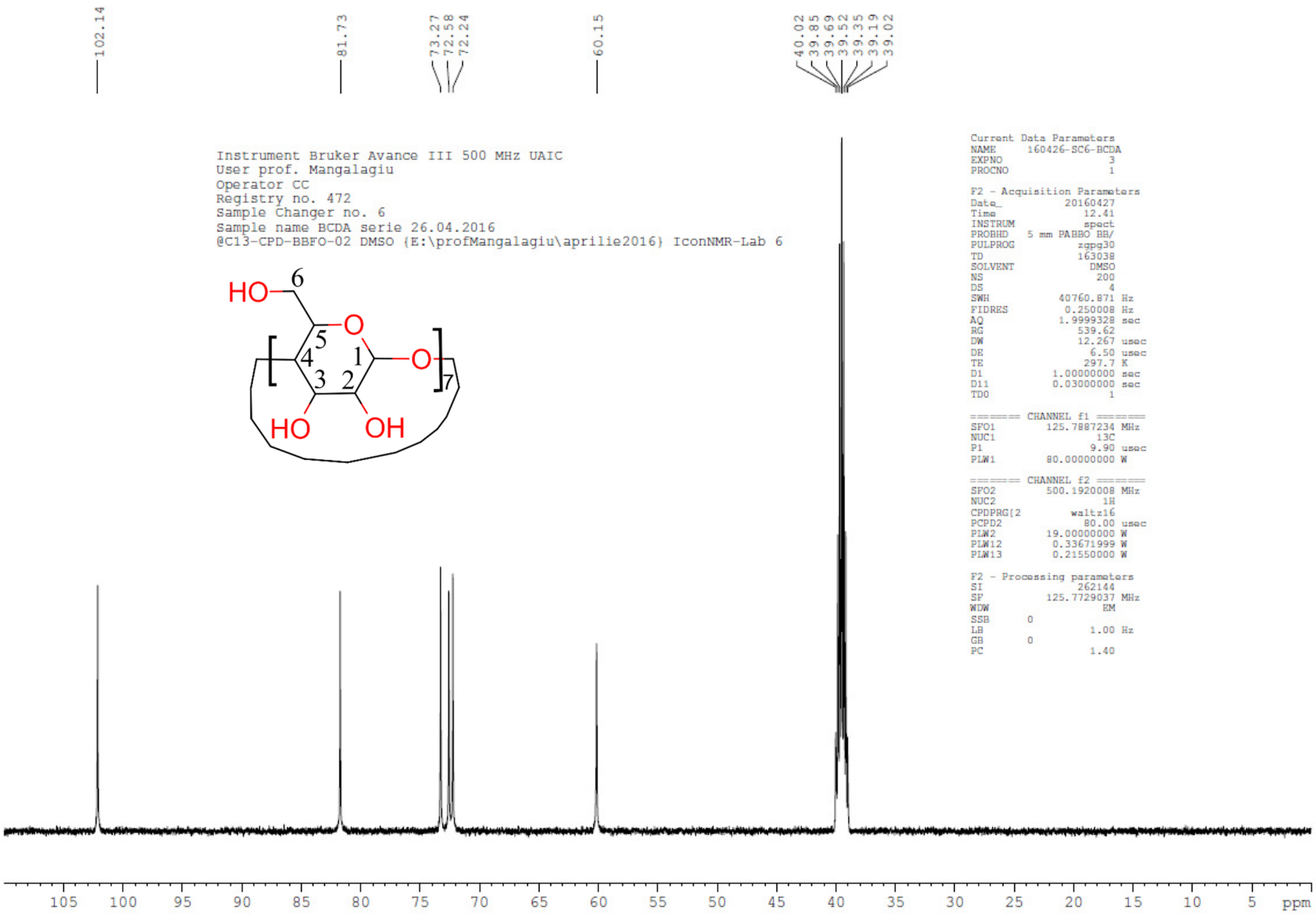

Figure S2. ^{13}C-NMR spectrum of β-CD

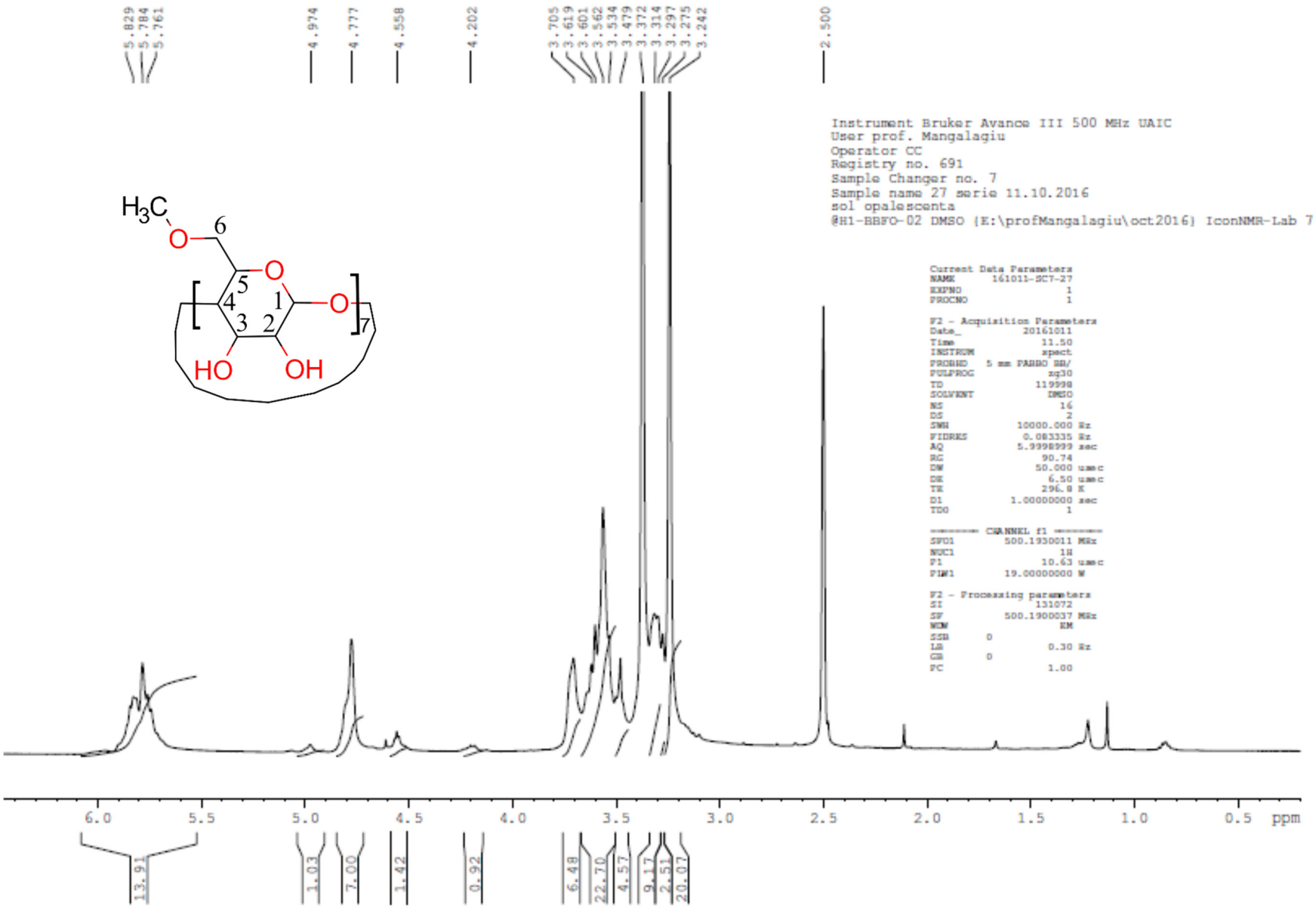

Figure S3. ^{1}H-NMR spectrum of MβCD

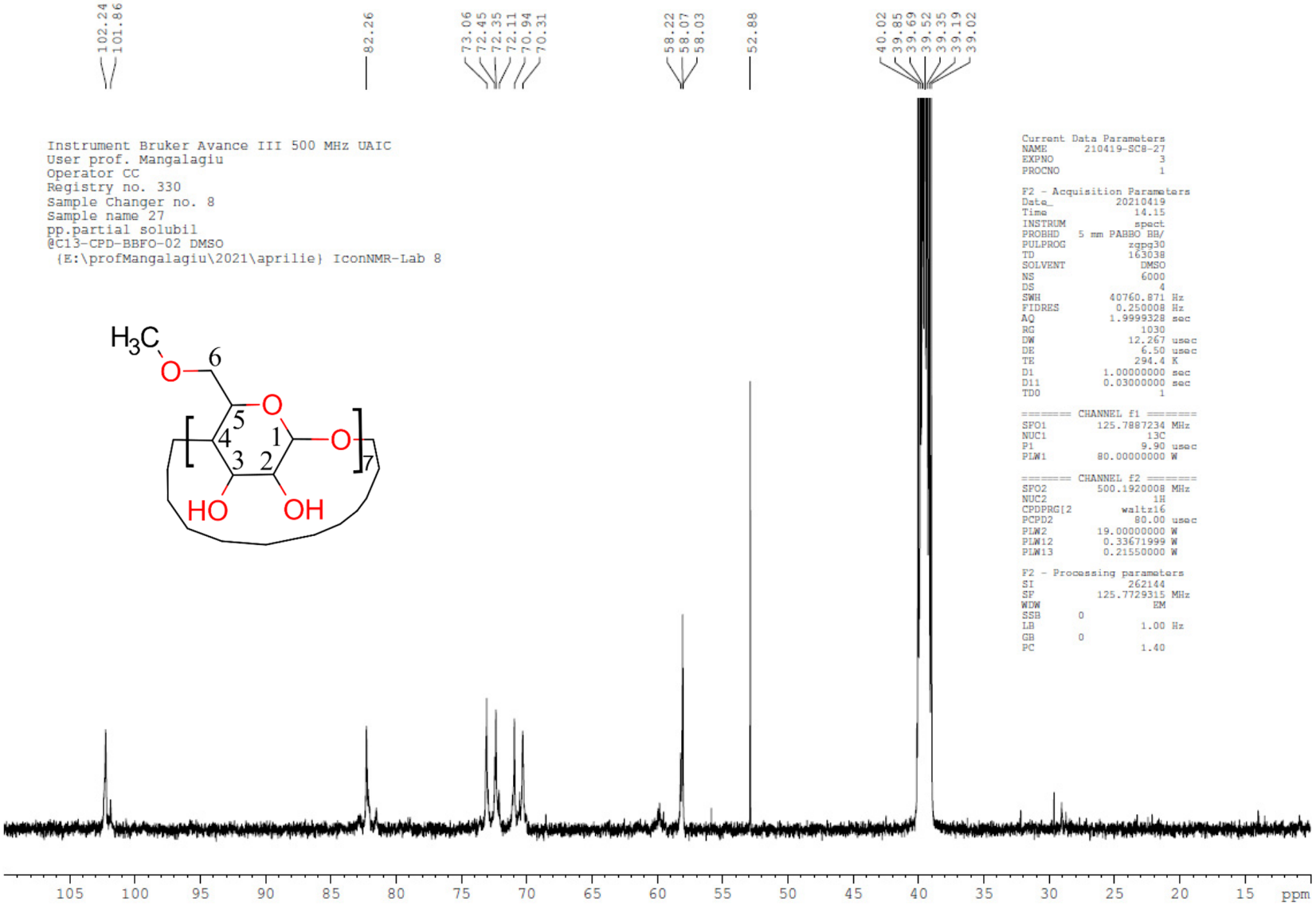

Figure S4. ^{13}C-NMR spectrum of MβCD

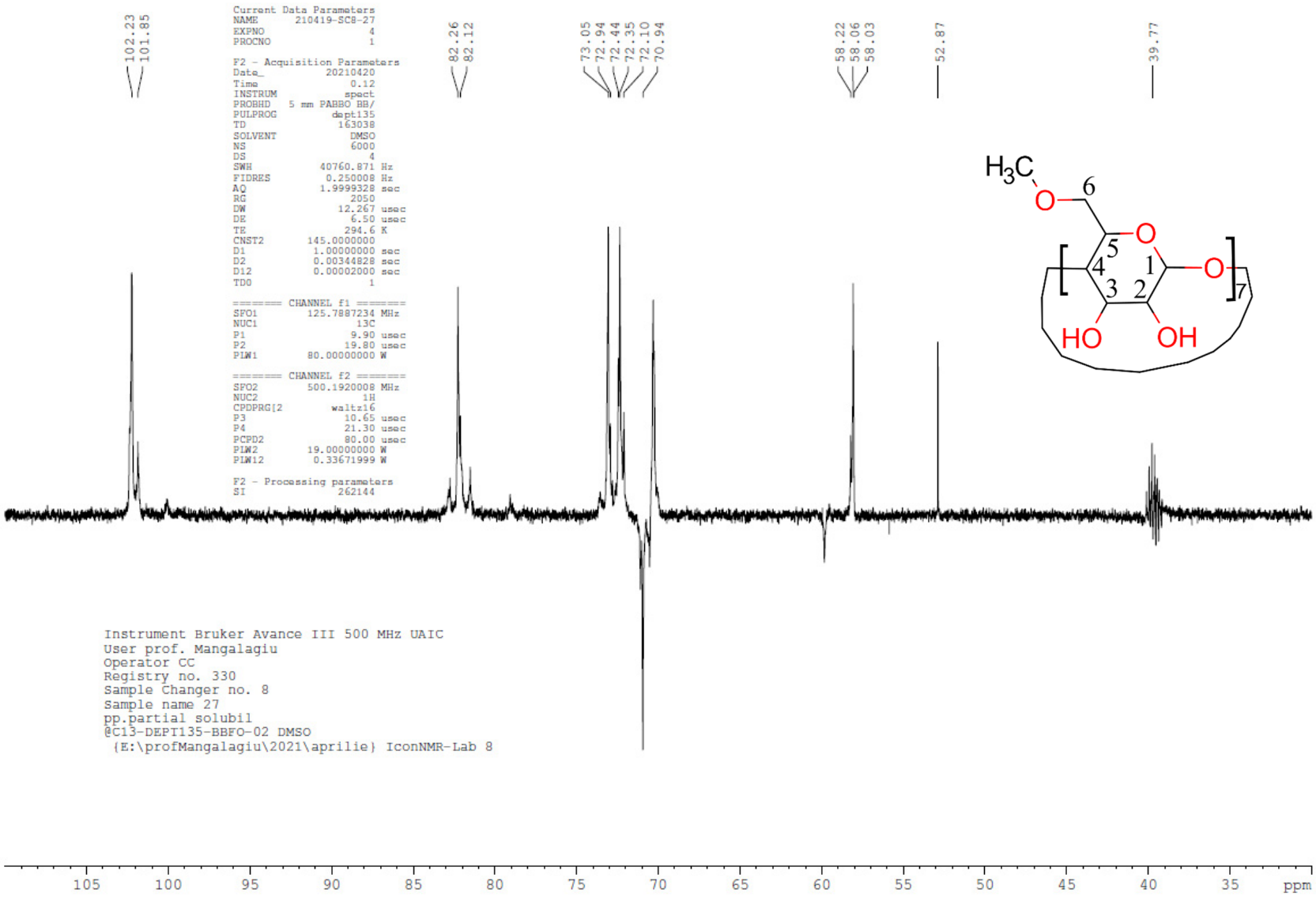

Figure S5. DEPT-135 ^{13}C-NMR spectrum MβCD

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Instrument Bruker Avance III 500 MHz UAIC
User prof. Mangalagiu
Operator CC
Registry no. 330
Sample Changer no. 8
Sample name 27
pp.partial solubil
@COSY45gs-BBFO-02 DMSO
 {E:\profMangalagiu\2021\aprilie} IconNMR-Lab 8
Current Data Parameters
NAME      210419-SC8-27
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_           20210420
Time                7.27
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG     cosygpqf45x
TD                 4096
SOLVENT            DMSO
NS                    2
DS                    8
SWH            8012.820 Hz
FIDRES         1.956255 Hz
AQ            0.2555904 sec
RG               835.64
DW               62.400 usec
DE                 6.50 usec
TE                293.7 K
D0            0.00000300 sec
D1            1.50000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012500 sec

======== CHANNEL f1 ========
SFO1        500.1930011 MHz
NUC1                  1H
P1                 10.63 usec
PLW1        19.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
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SFO1             500.193 MHz
FIDRES        15.625000 Hz
SW               15.994 ppm
FnMODE               QF

F2 - Processing parameters
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SF          500.1900019 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
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WDW                QSINE
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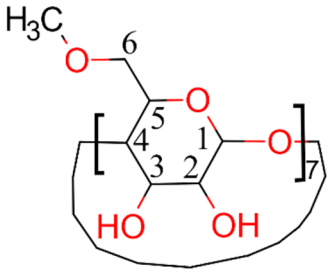

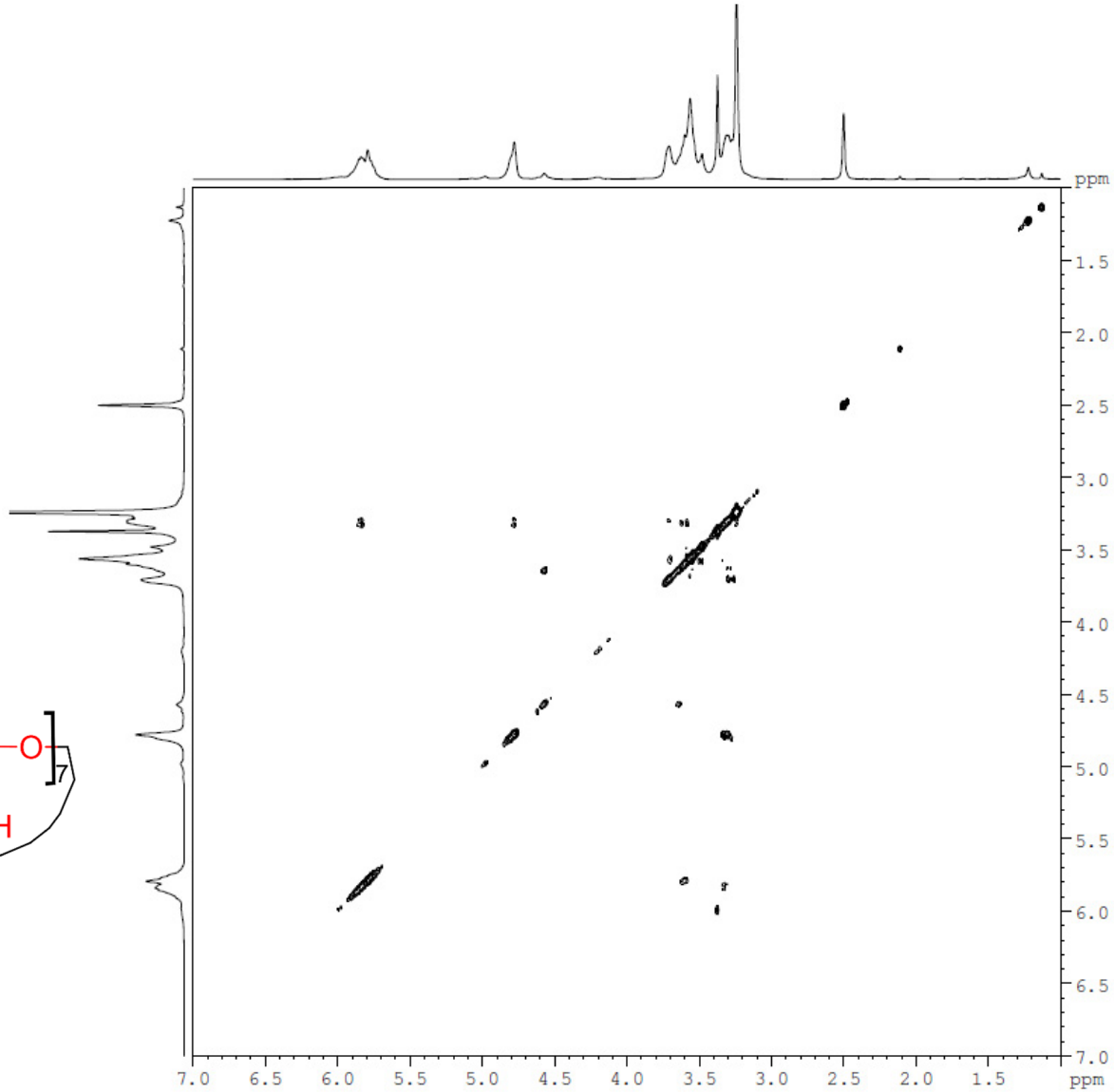

Figure S6. COSY NMR spectrum MβCD

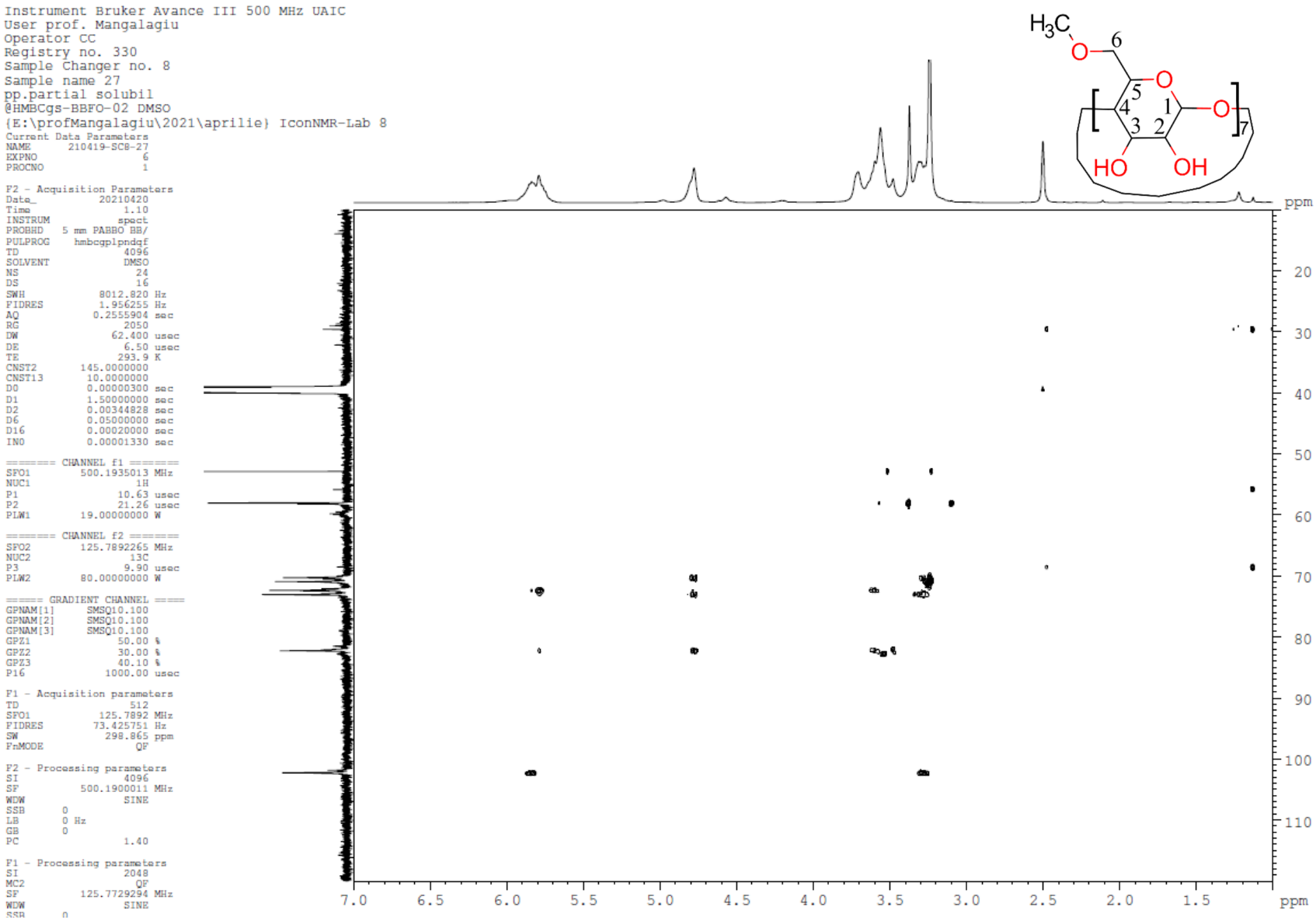

Figure S7. HMBC NMR spectrum MβCD

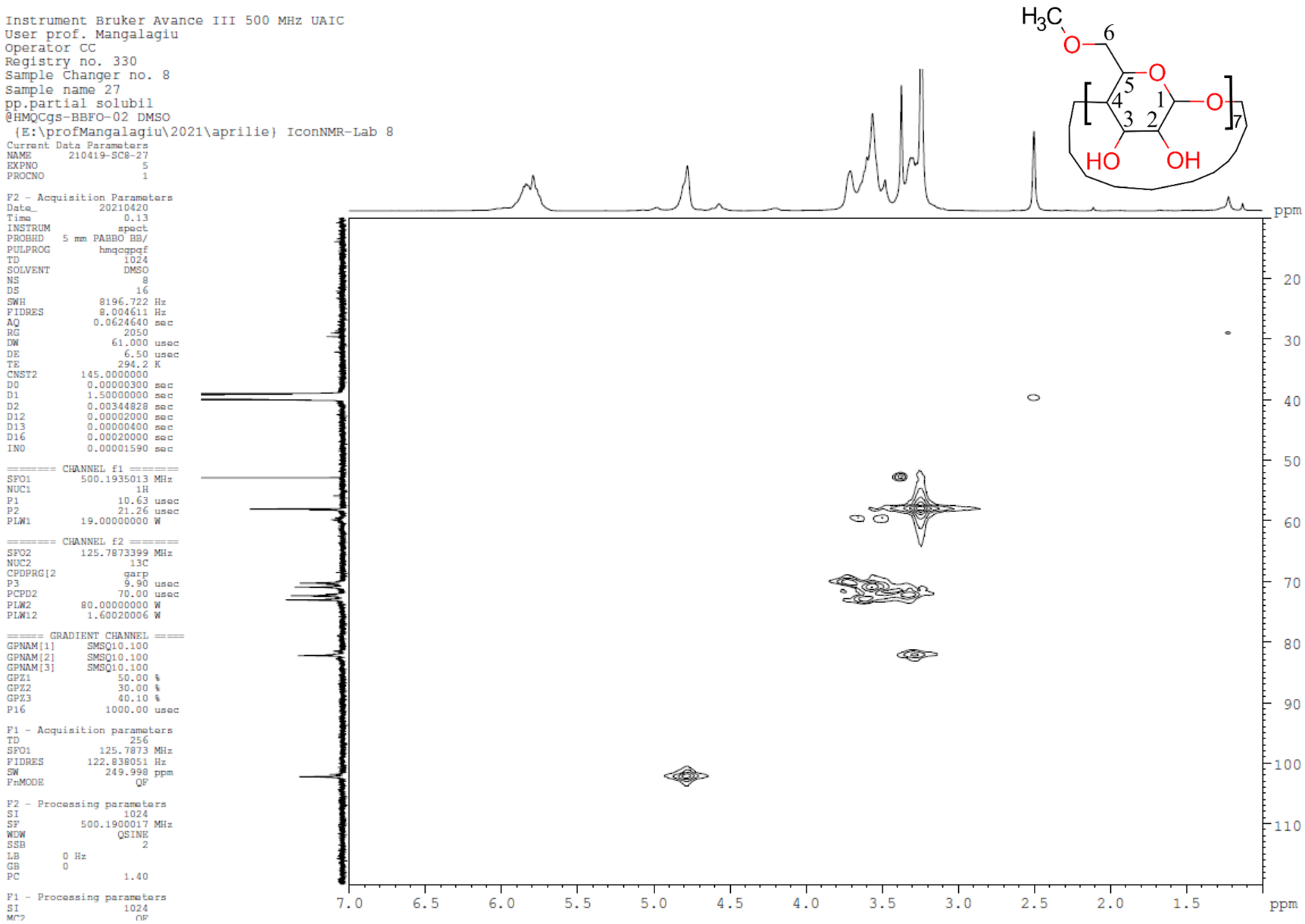

Figure S8. HMQC NMR spectrum MβCD

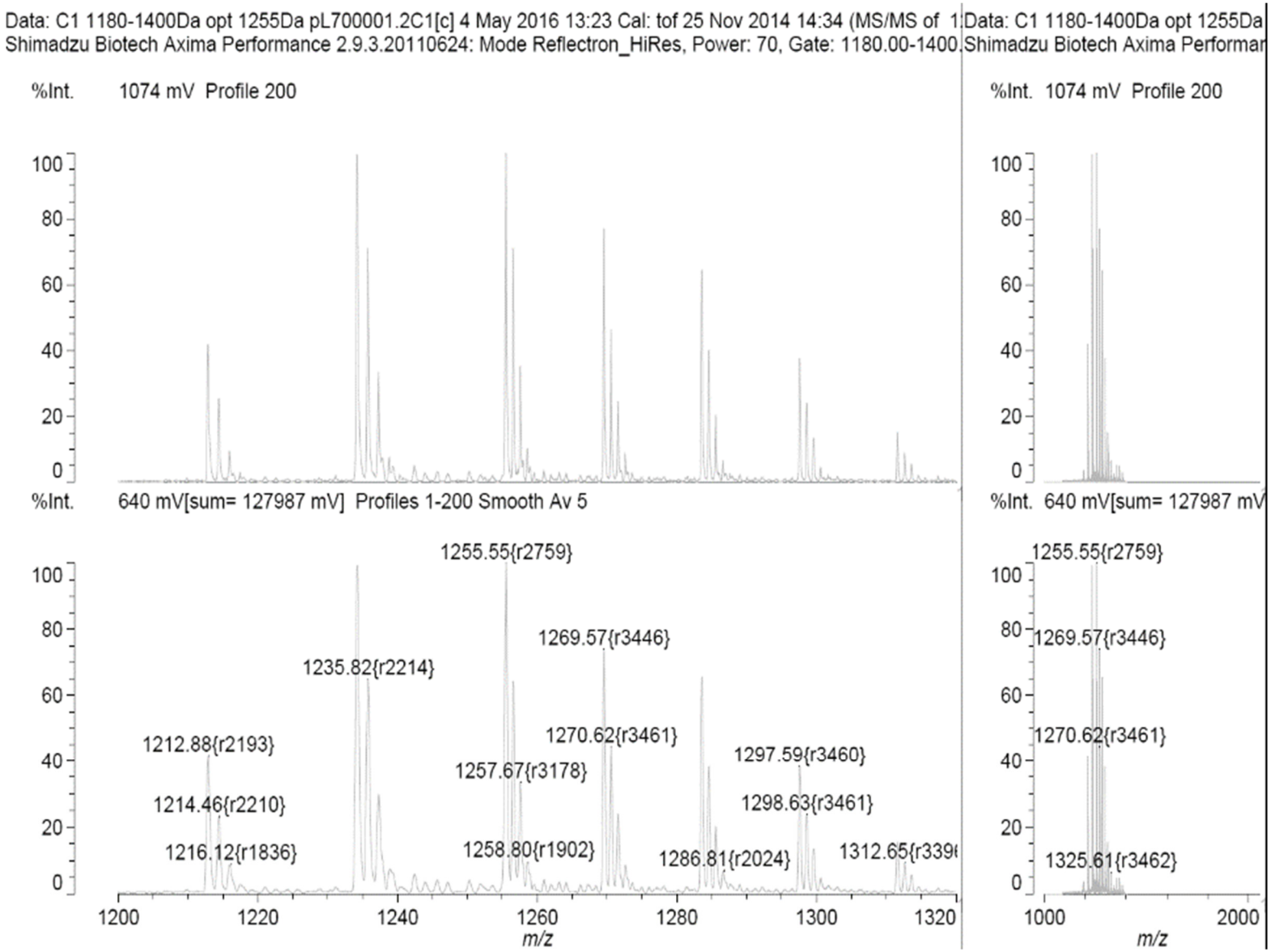

Figure S9. MALDI-TOF spectrum of MβCD

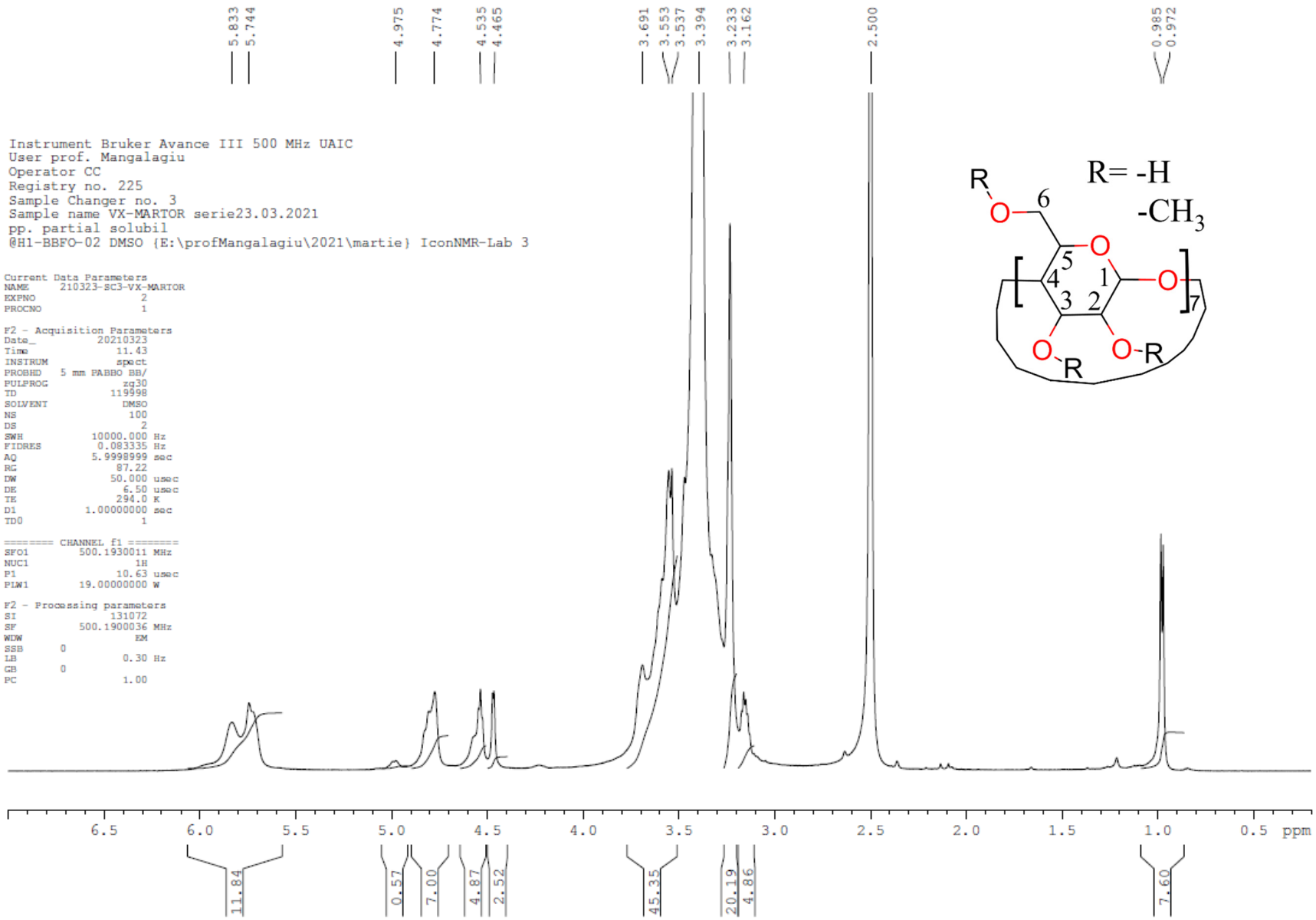

Figure S10. ^{1}H-NMR spectrum of Reference sample

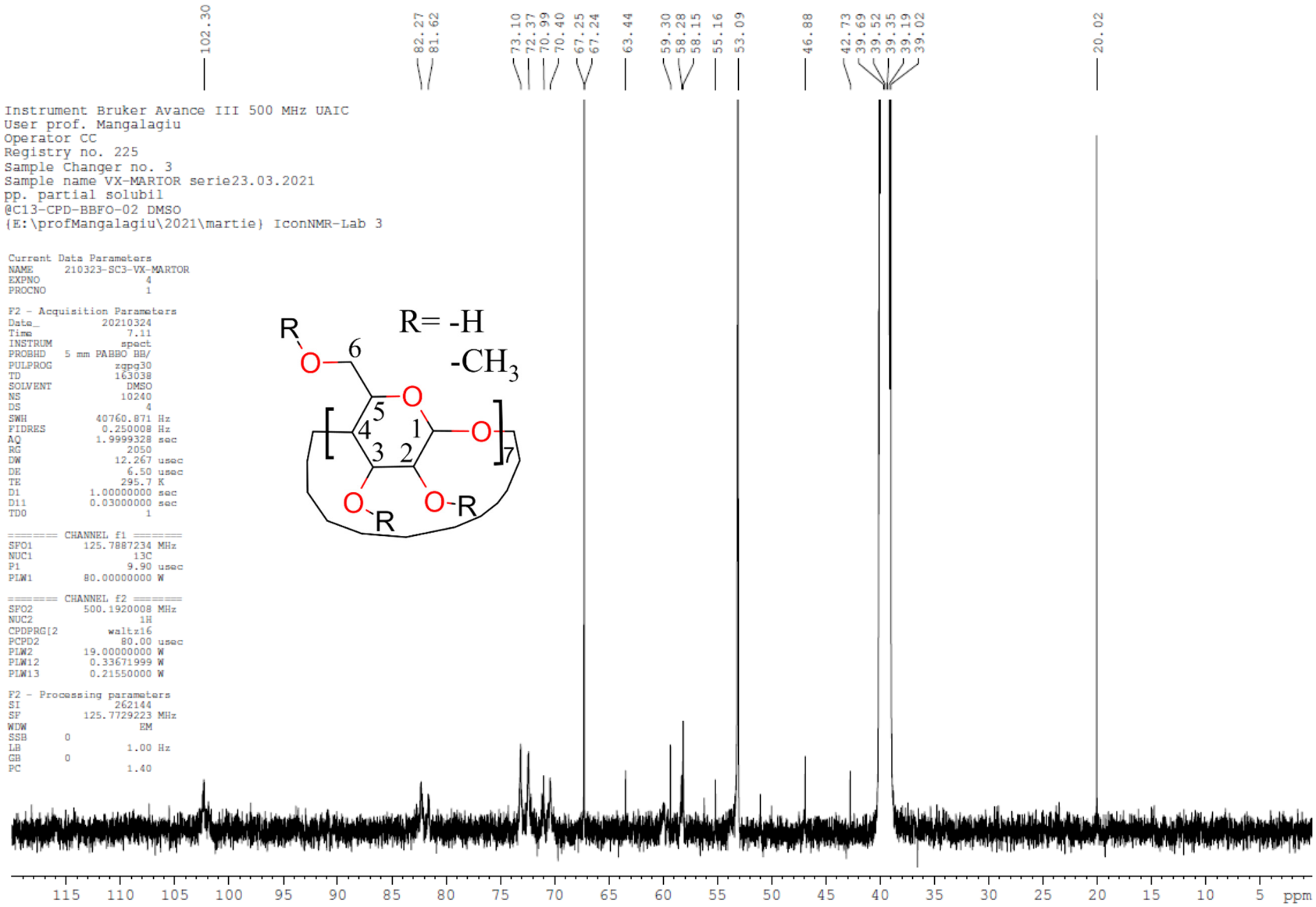

Figure S11. ^{13}C-NMR spectrum of Reference sample

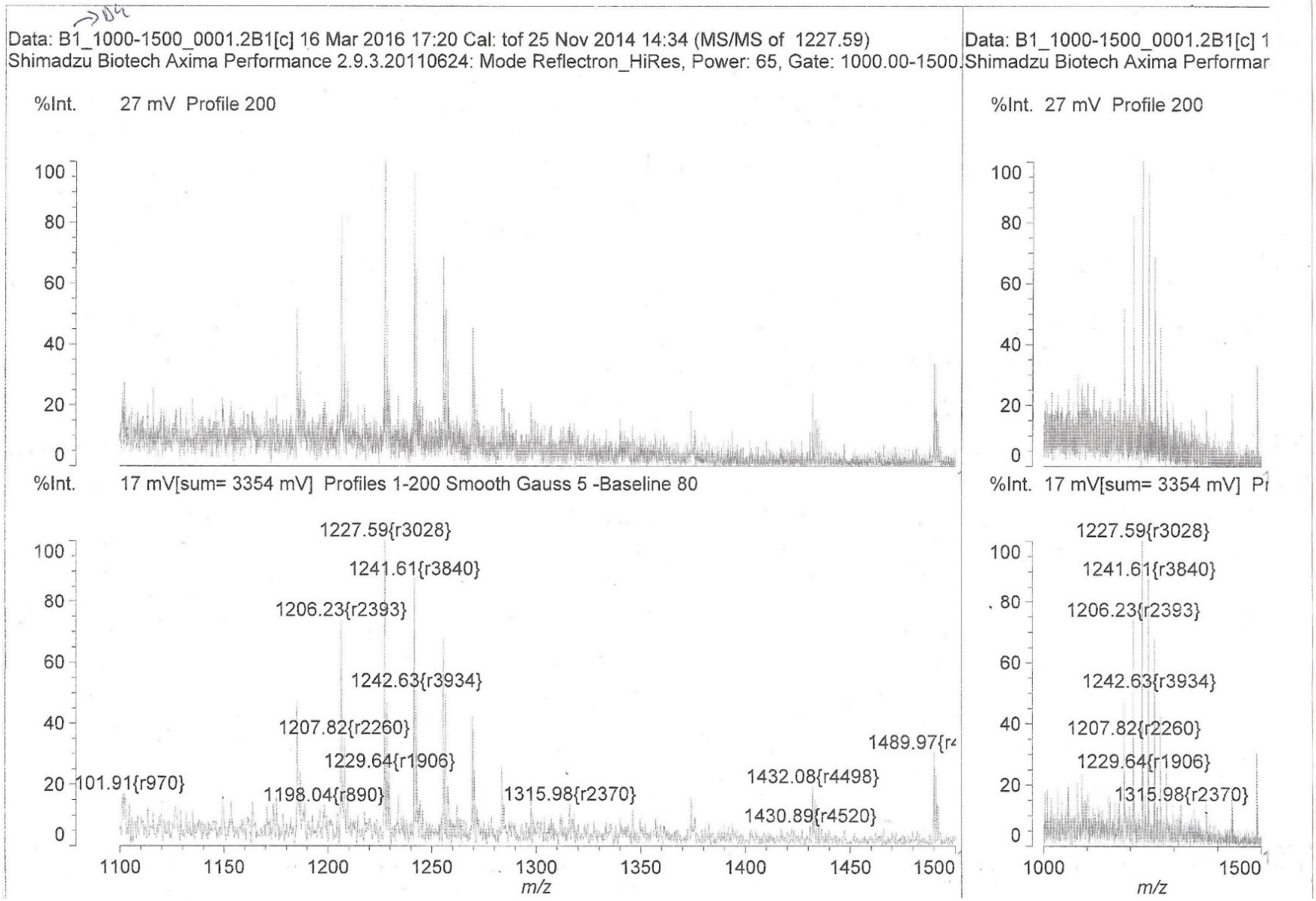

Figure S12. MALDI-TOF spectrum of Reference sample

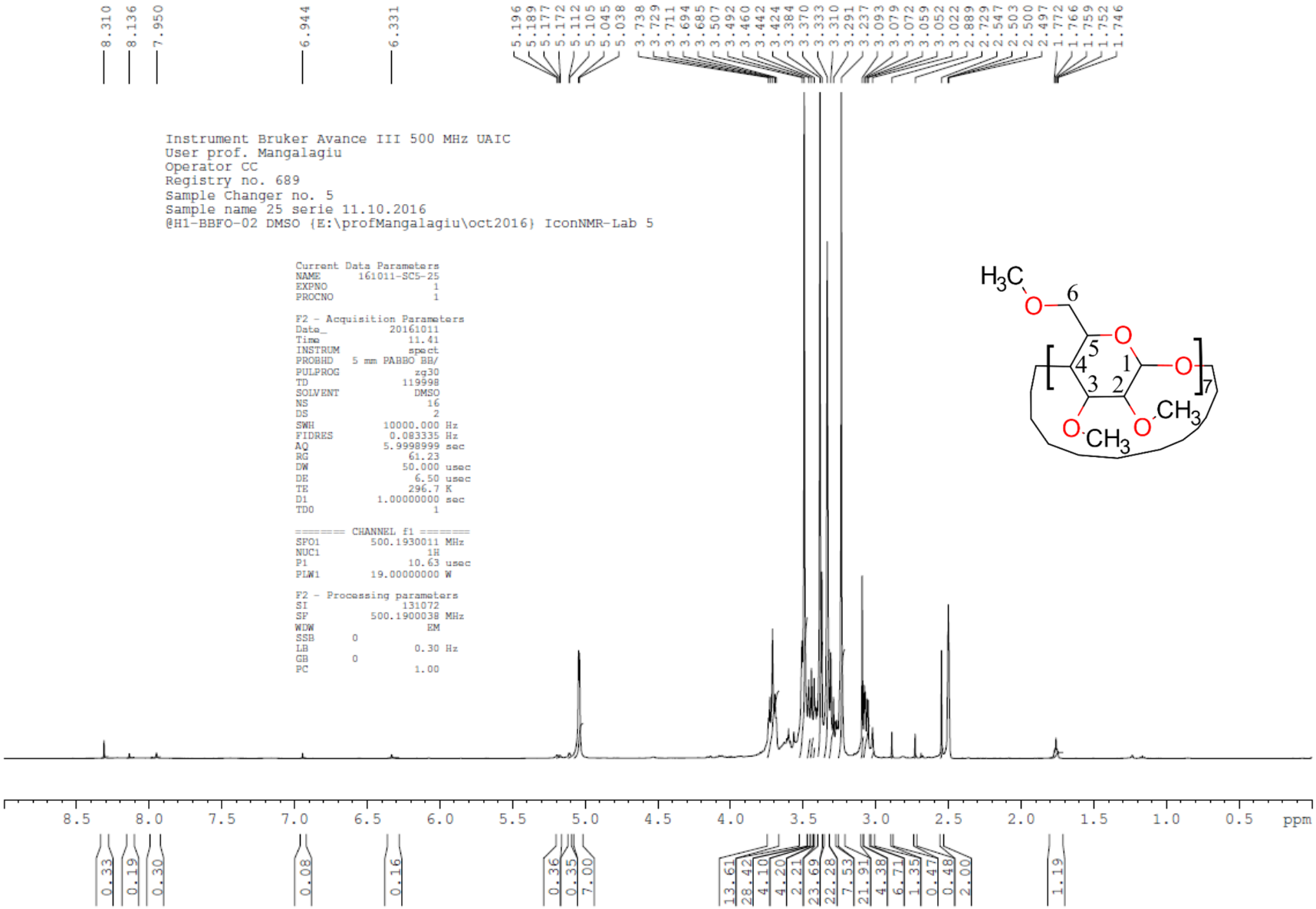

Figure S13. ^{1}H-NMR spectrum of TRIMEB

Table S1. Calculated masses for methylated regioisomers of *β*-CD

CH_3 Groups	Molecular Formula	Monoisotopic Mass	M+H	M+Na	M+K	M+NH4
0 (*β*-CD)	C42H70O35	1134.369764	1135.377589	**1157.359533**	1173.33347	1152.404138
1	C43H72O35	1148.385414	1149.393239	**1171.375183**	1187.34912	1166.419788
2	C44H74O35	1162.401064	1163.408889	**1185.390833**	1201.364771	1180.435438
3	C45H76O35	1176.416714	1177.424539	**1199.406483**	1215.380421	1194.451088
4	C46H78O35	1190.432364	1191.440189	**1213.422133**	1229.396071	1208.466738
5	C47H80O35	1204.448014	1205.455839	**1227.437784**	1243.411721	1222.482388
6	C48H82O35	1218.463664	1219.471489	**1241.453434**	1257.427371	1236.498038
7 (M*β*CD)	C49H84O35	1232.479314	1233.487139	**1255.469084**	1271.443021	1250.513689
8	C50H86O35	1246.494964	1247.502789	**1269.484734**	1285.458671	1264.529339
9	C51H88O35	1260.510615	1261.51844	**1283.500384**	1299.474321	1278.544989
10	C52H90O35	1274.526265	1275.53409	**1297.516034**	1313.489971	1292.560639
11	C53H92O35	1288.541915	1289.54974	**1311.531684**	1327.505621	1306.576289
12	C54H94O35	1302.557565	1303.56539	**1325.547334**	1341.521271	1320.591939
13	C55H96O35	1316.573215	1317.58104	**1339.562984**	1355.536921	1334.607589
14 DIMEB	C56H98O35	1330.588865	1331.59669	**1353.578634**	1369.552571	1348.623239
15	C57H100O35	1344.604515	1345.61234	**1367.594284**	1383.568221	1362.638889
16	C58H102O35	1358.620165	1359.62799	**1381.609934**	1397.583871	1376.654539
17	C59H104O35	1372.635815	1373.64364	**1395.625584**	1411.599522	1390.670189
18	C60H106O35	1386.651465	1387.65929	**1409.641234**	1425.615172	1404.685839
19	C61H108O35	1400.667115	1401.67494	**1423.656884**	1439.630822	1418.701489
20	C62H110O35	1414.682765	1415.69059	**1437.672535**	1453.646472	1432.717139
21 TRIMEB	C63H112O35	1428.698415	1429.70624	**1451.688185**	1467.662122	1446.732789