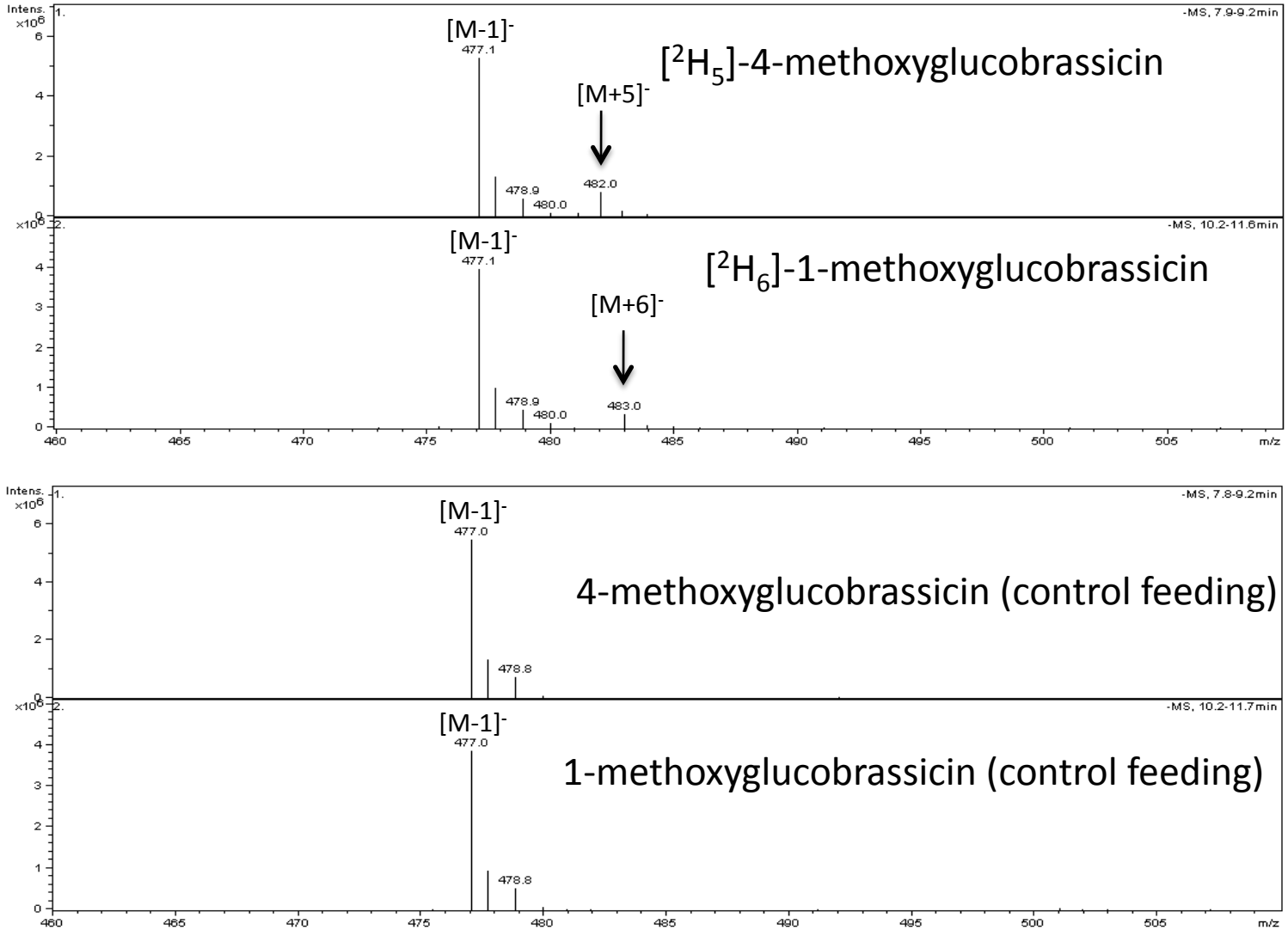
Appendix A. Supplementary data

Unveiling the phytoalexin biosynthetic puzzle in salt cress: Unprecedented incorporation of glucobrassicin into wasalexins A and B

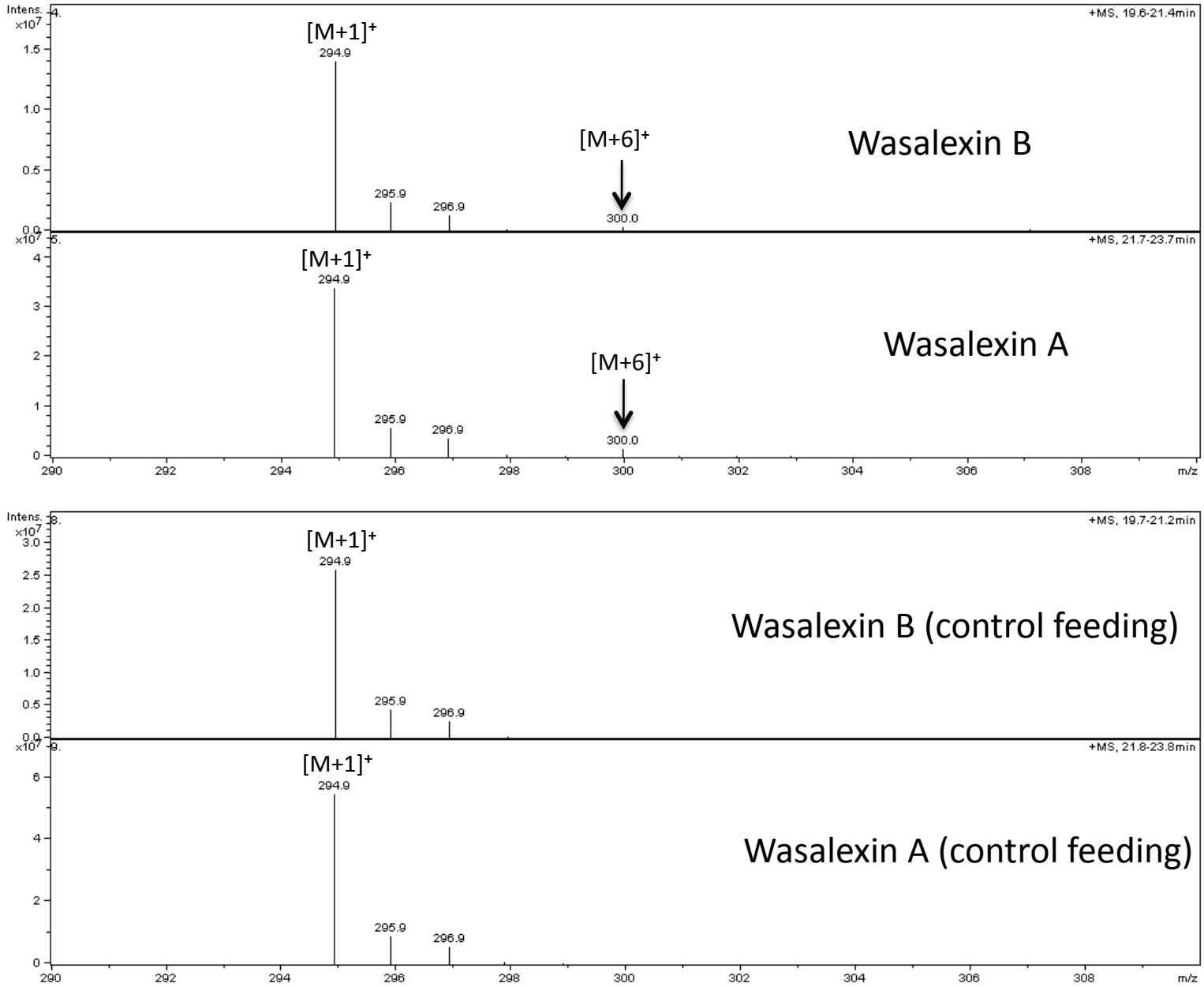
M. Soledade C. Pedras,* Estifanos E. Yaya and Sajjad Hossain
Department of Chemistry, University of Saskatchewan, 110 Science Place,
Saskatoon, SK, S7N 5C9,
Canada

Corresponding author: M. Soledade C. Pedras
Email: s.pedras@usask.ca;
Telephone: 1-306- 966-4772;
Fax: 1-306-966-4730

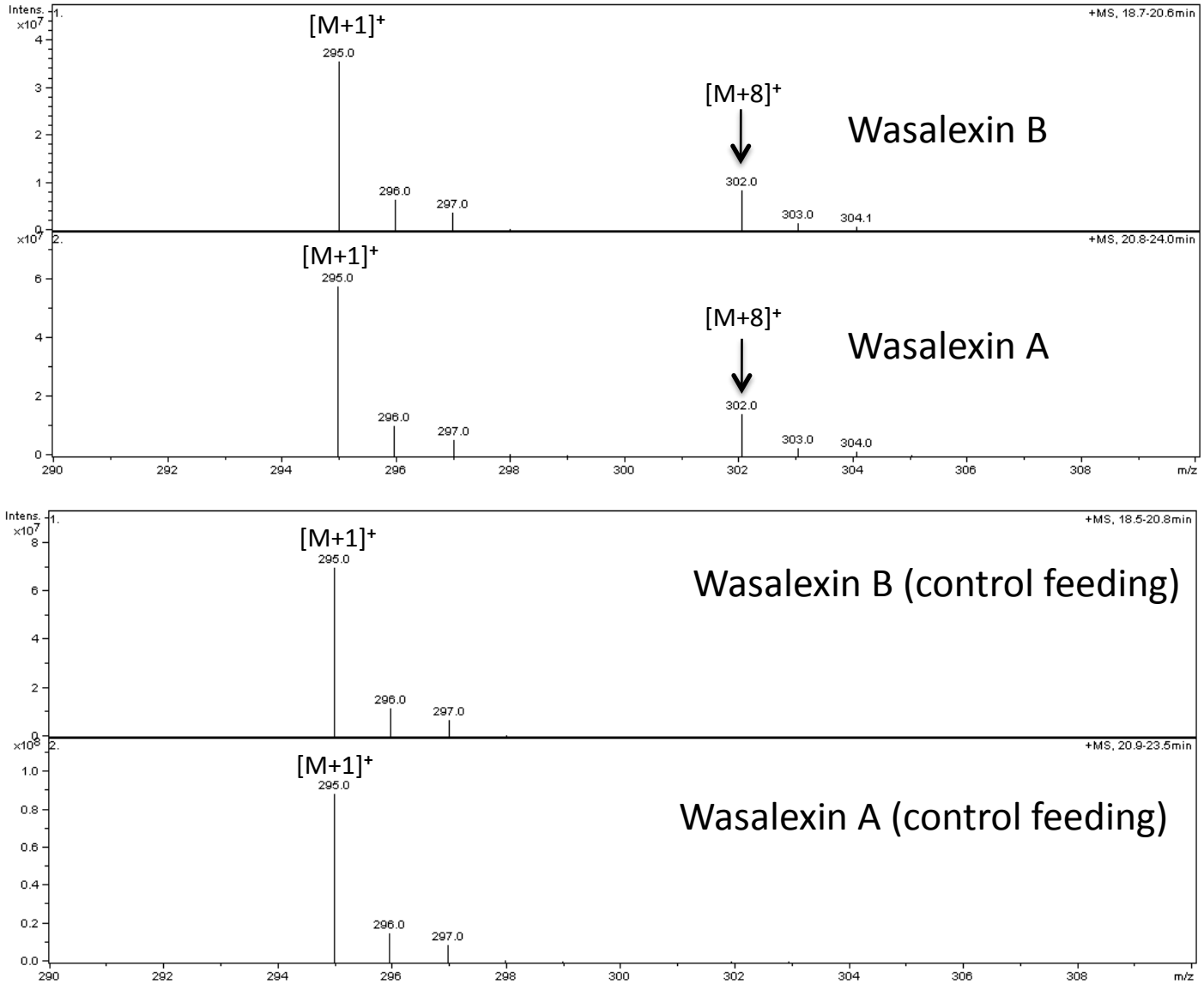
MS-ESI of [2,2,4',5',6',7'-$^2H_6$]glucobrassicin (**12a**) feedings and control feedings

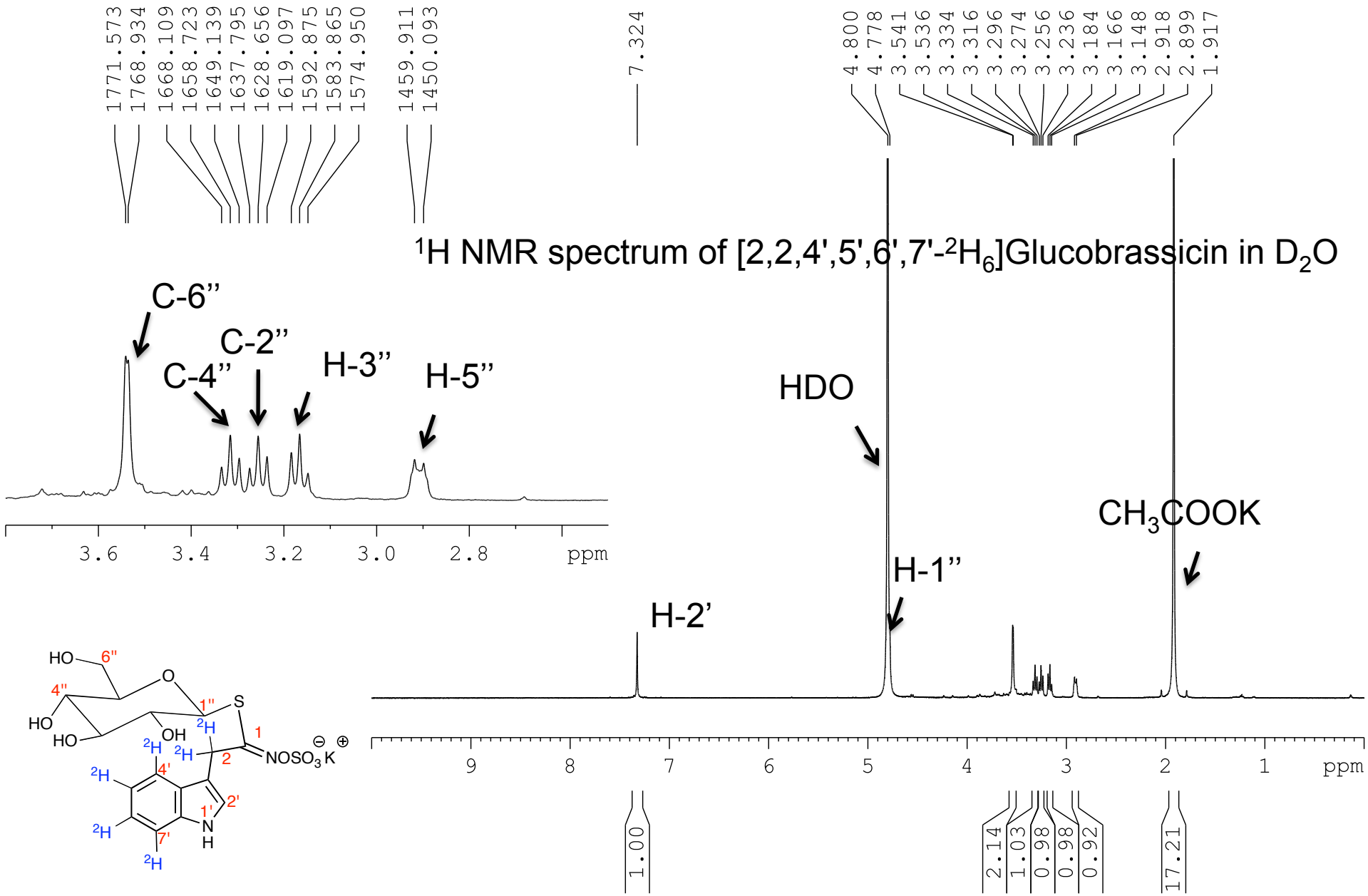


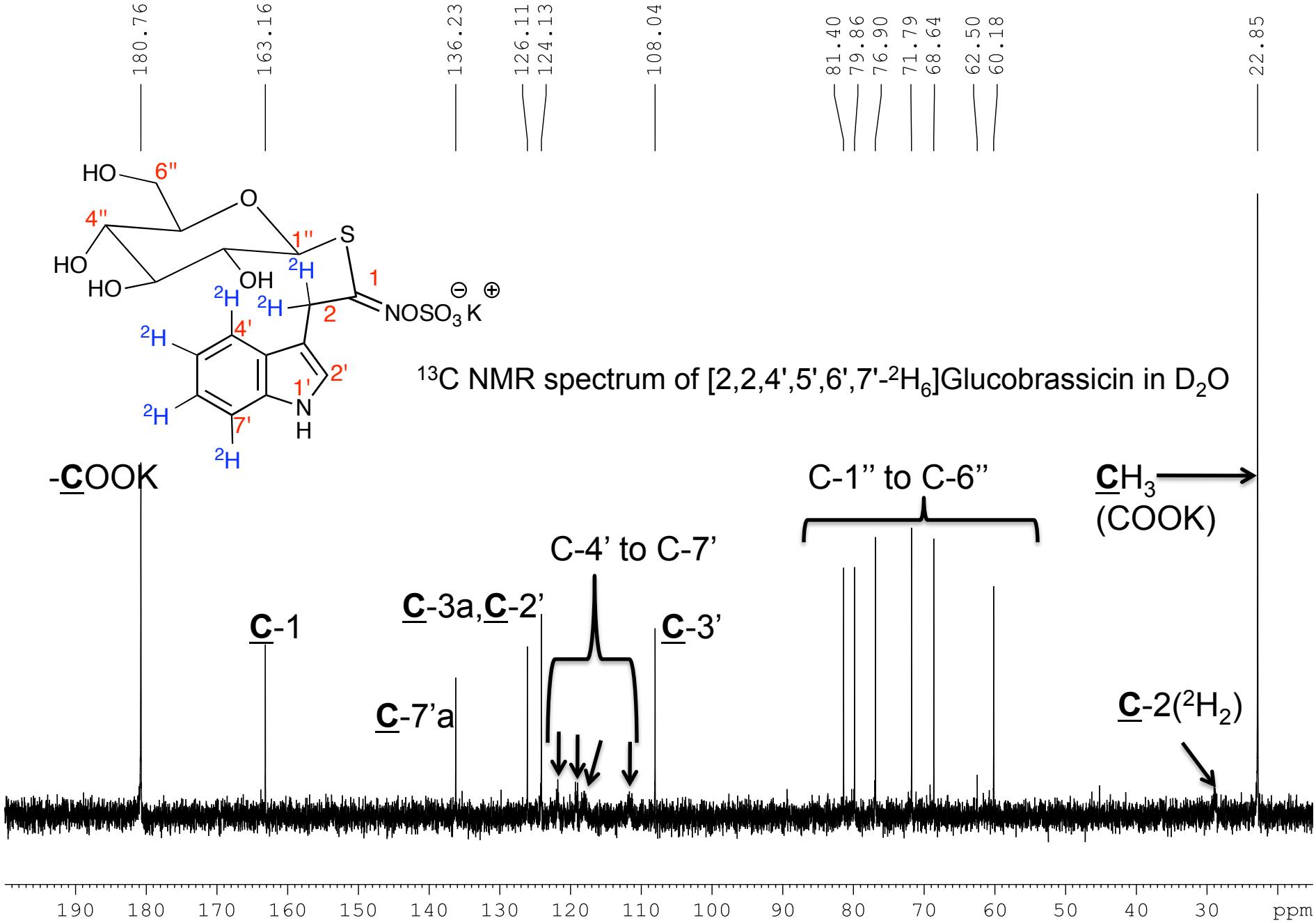
MS-ESI of [2,2,4',5',6',7'-$^{2}H_{6}$]glucobrassicin (**12a**) feedings and control feedings



MS-ESI of [^2H_3C-S 4',5',6',7'-$^2H_4$]-1-methoxybrassinin (**6a**) feedings and control feedings

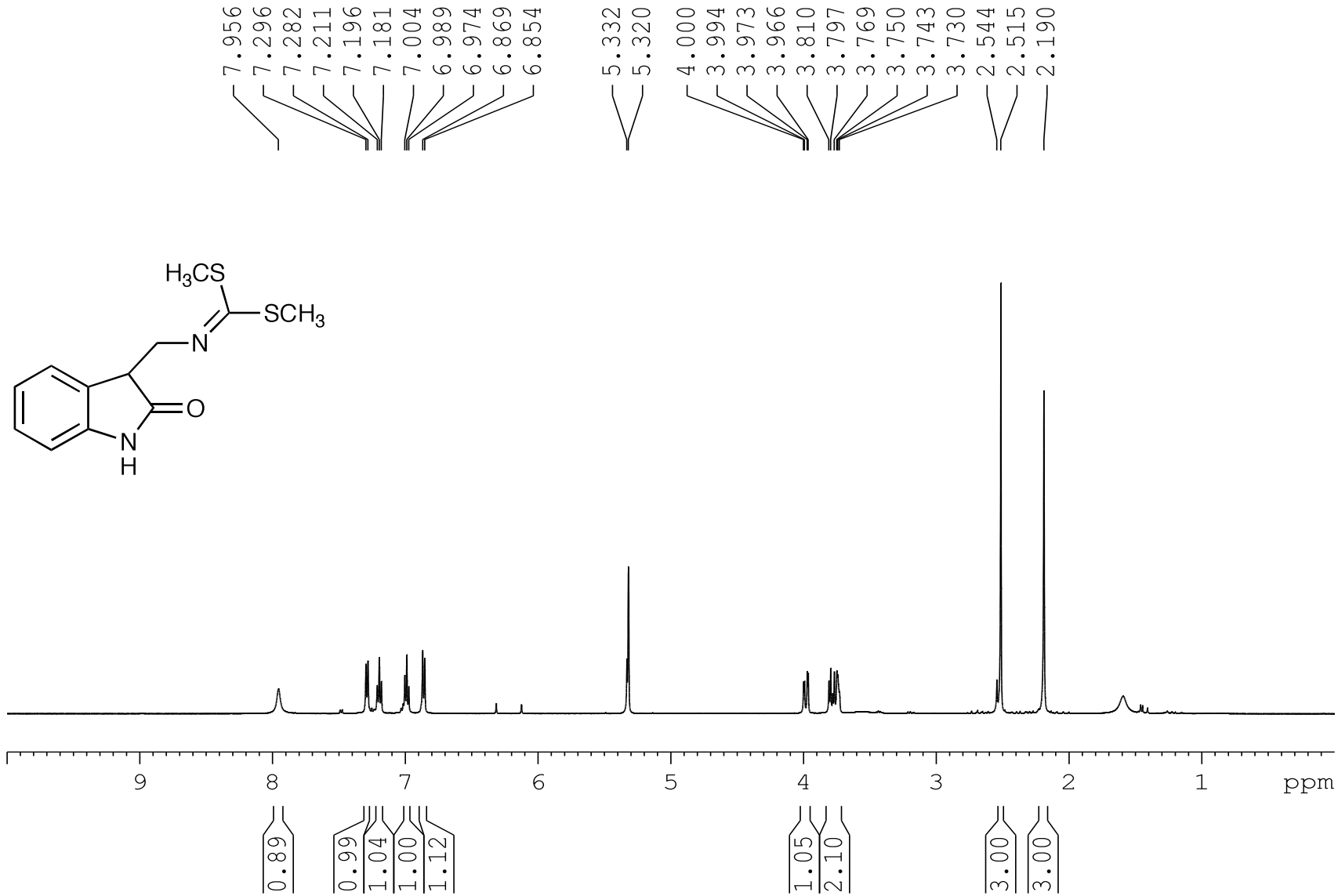



1771.573
1768.934
1668.109
1658.723
1649.139
1637.795
1628.656
1619.097
1592.875
1583.865
1574.950
1459.911
1450.093
7.324
4.800
4.778
3.541
3.536
3.334
3.316
3.296
3.274
3.256
3.236
3.184
3.166
3.148
2.918
2.899
1.917
^{1}H NMR spectrum of [2,2,4',5',6',7'-$^2H_6$]Glucobrassicin in D_2O
C-6''
C-2''
C-4''
H-3''
H-5''
HDO
H-1''
H-2'
CH_3COOK
3.6
3.4
3.2
3.0
2.8
ppm
9
8
7
6
5
4
3
2
1
ppm
1.00
2.14
1.03
0.98
0.98
0.92
17.21
HO
6''
O
4''
1''
S
HO
HO
OH
^2H
1
2
$NOSO_3K$
4'
2'
1'
N
H
7'

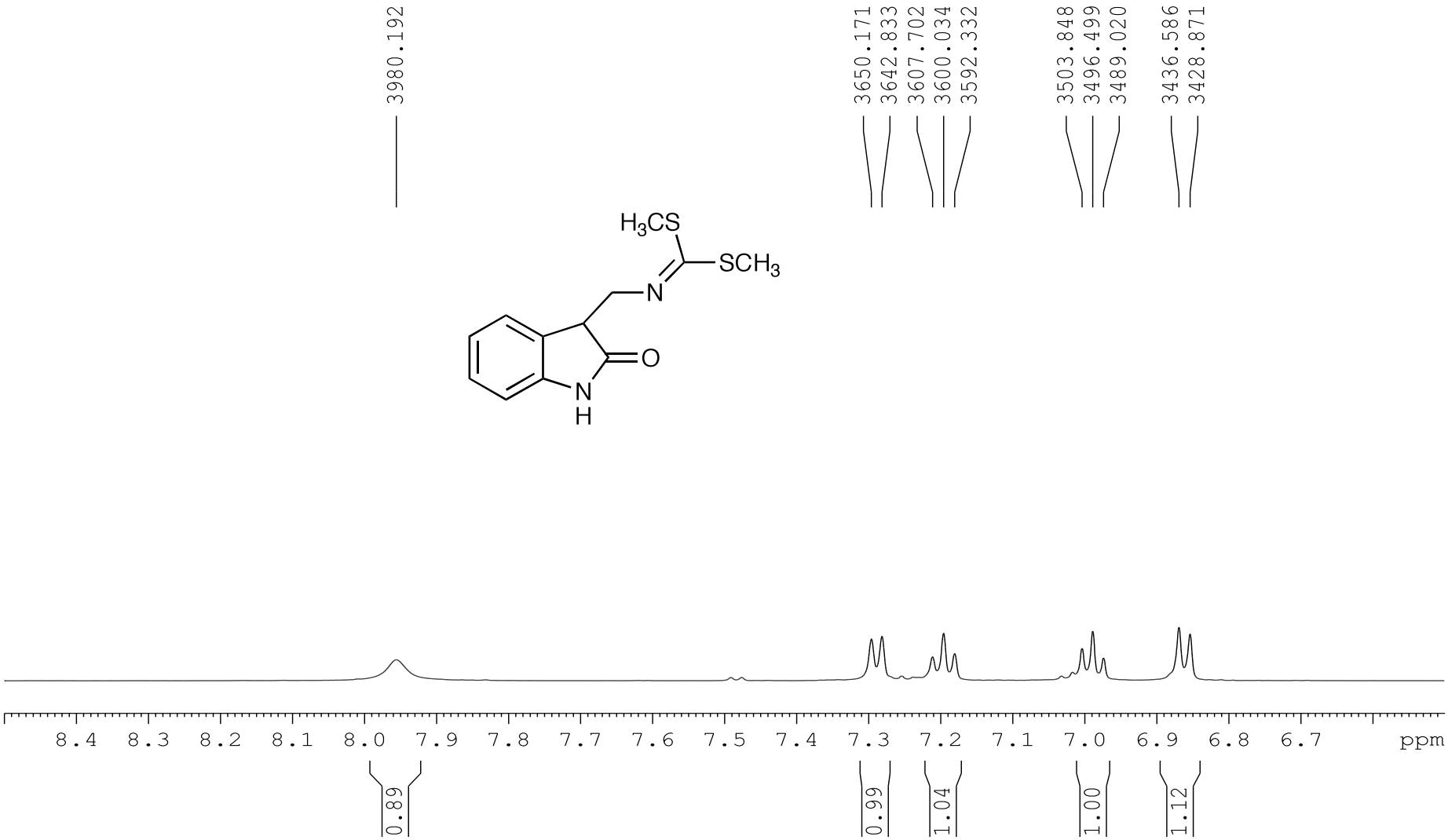


^{13}C NMR spectrum of [2,2,4',5',6',7'-$^{2}H_6$]Glucobrassicin in D_2O

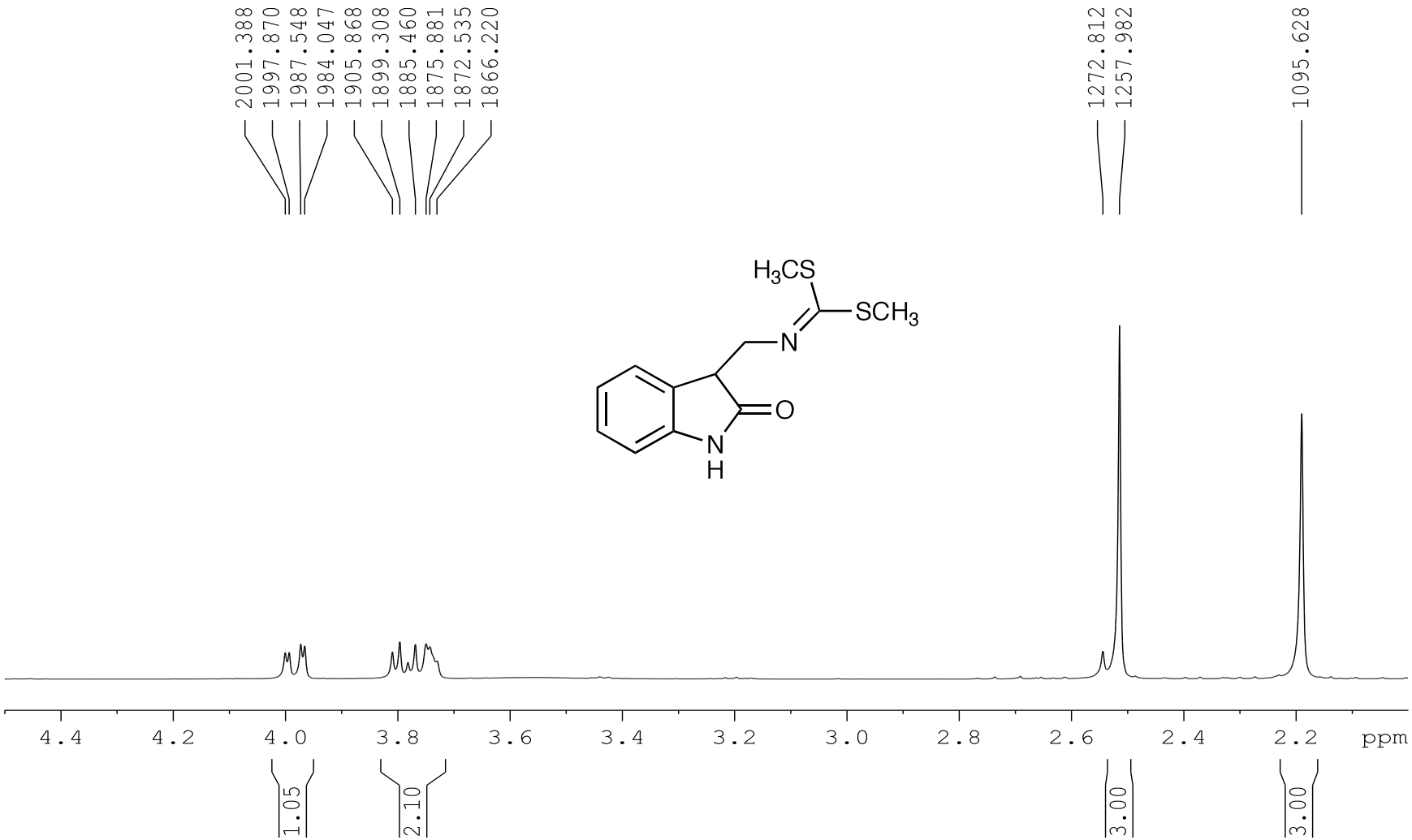
Demethoxydihydrowasalexin - ^{1}H NMR (CD_2Cl_2)



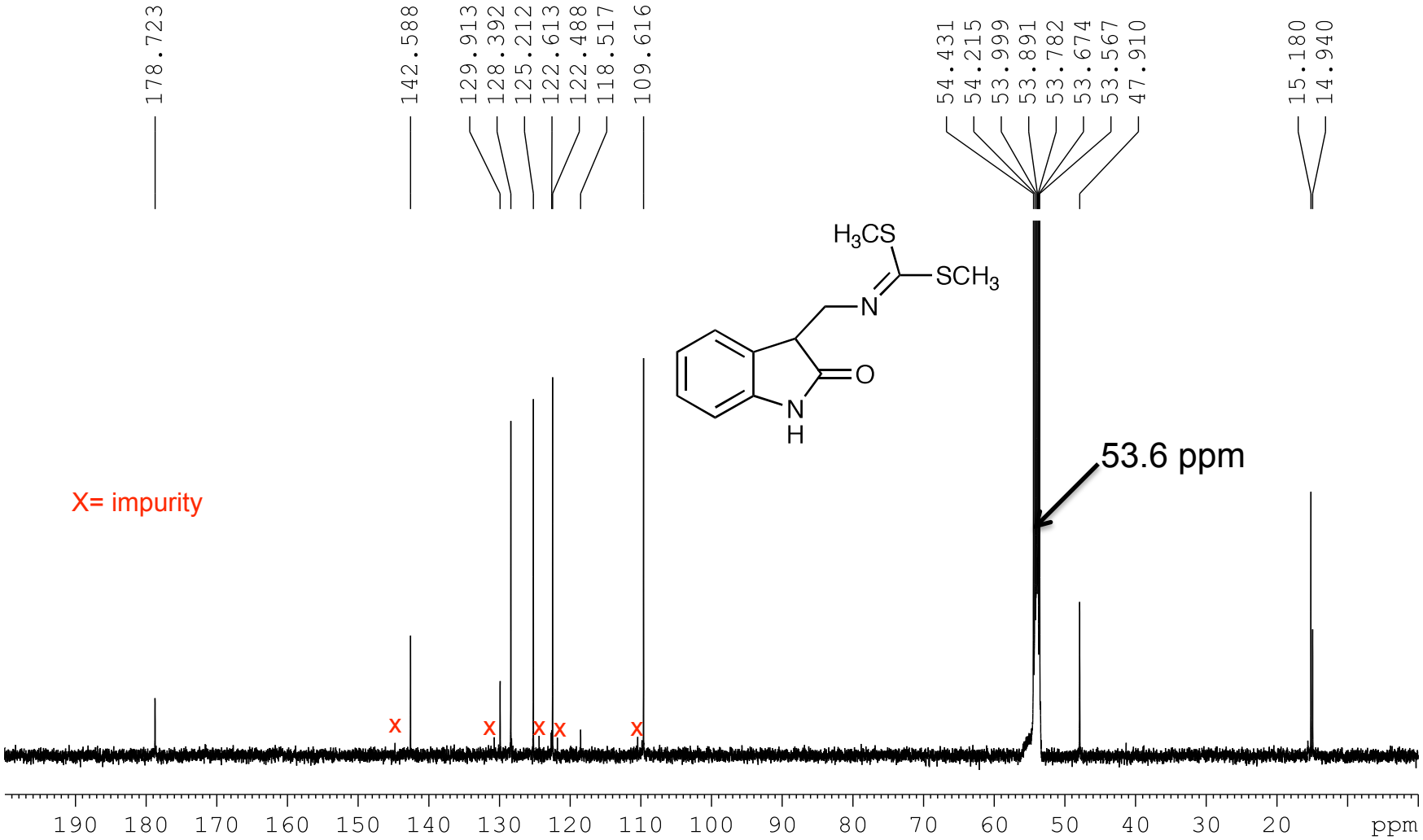
Demethoxydihydrowasalexin - ^{1}H NMR (CD_2Cl_2)



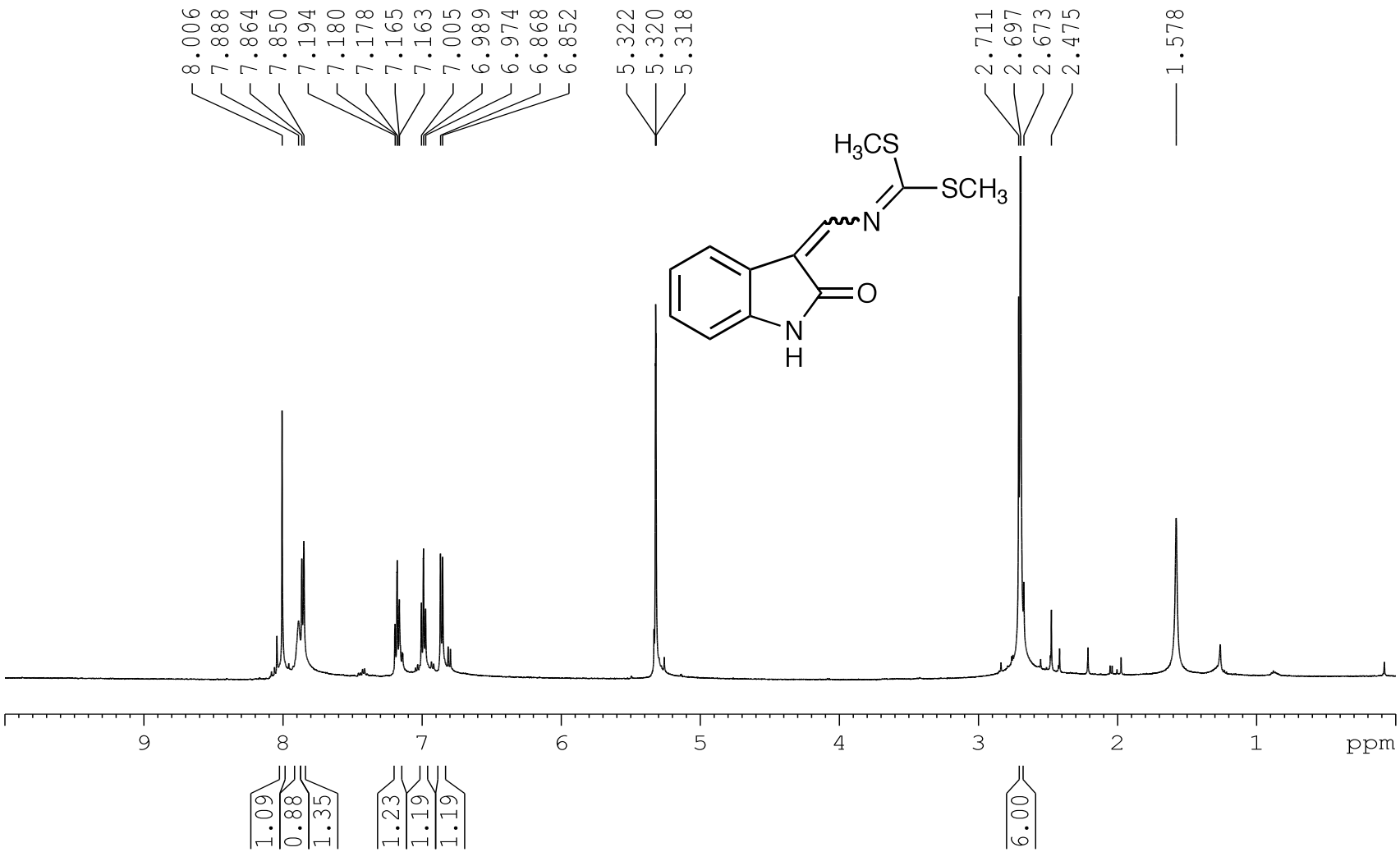
Demethoxydihydrowasalexin - ^{1}H NMR (CD_2Cl_2)



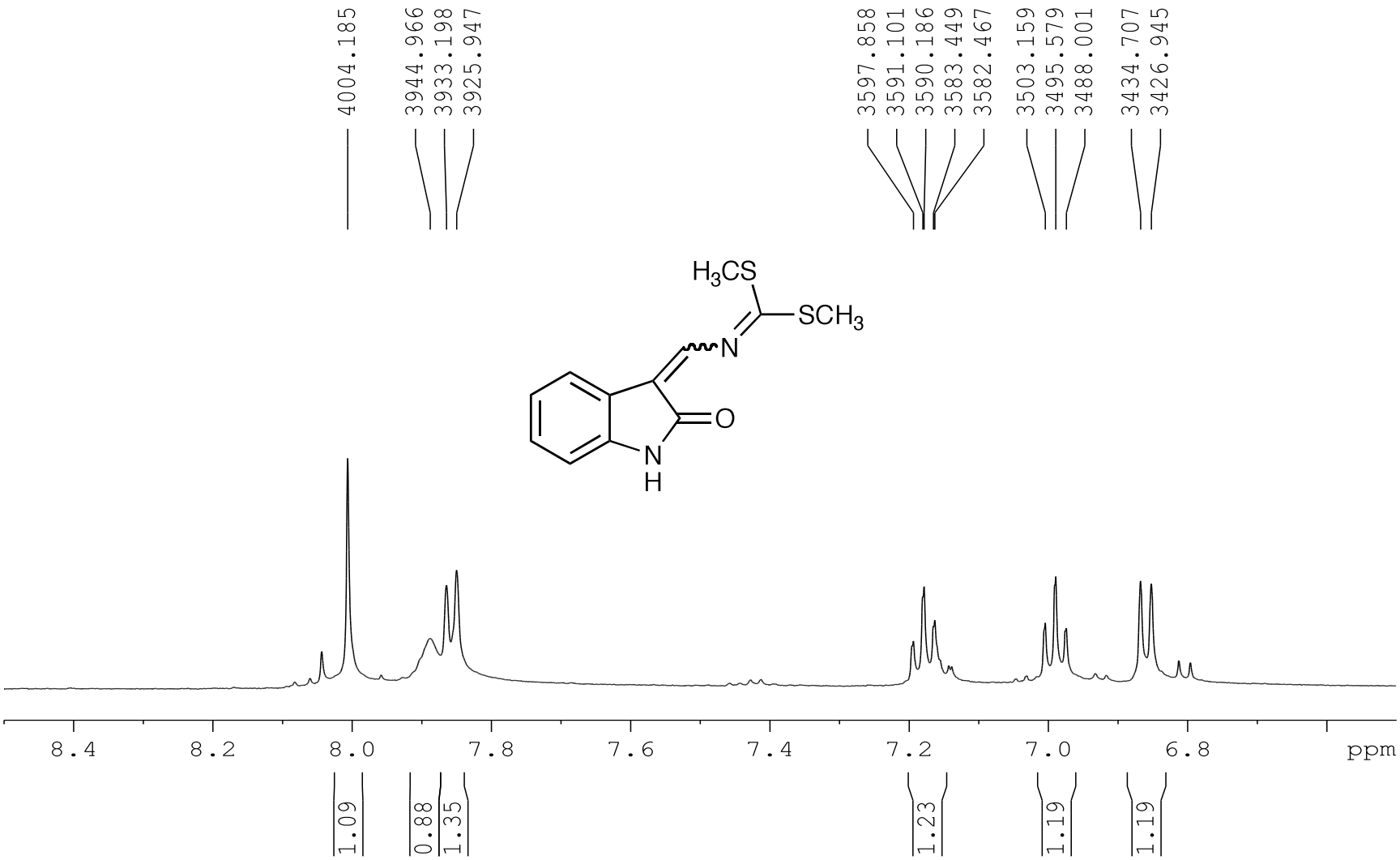
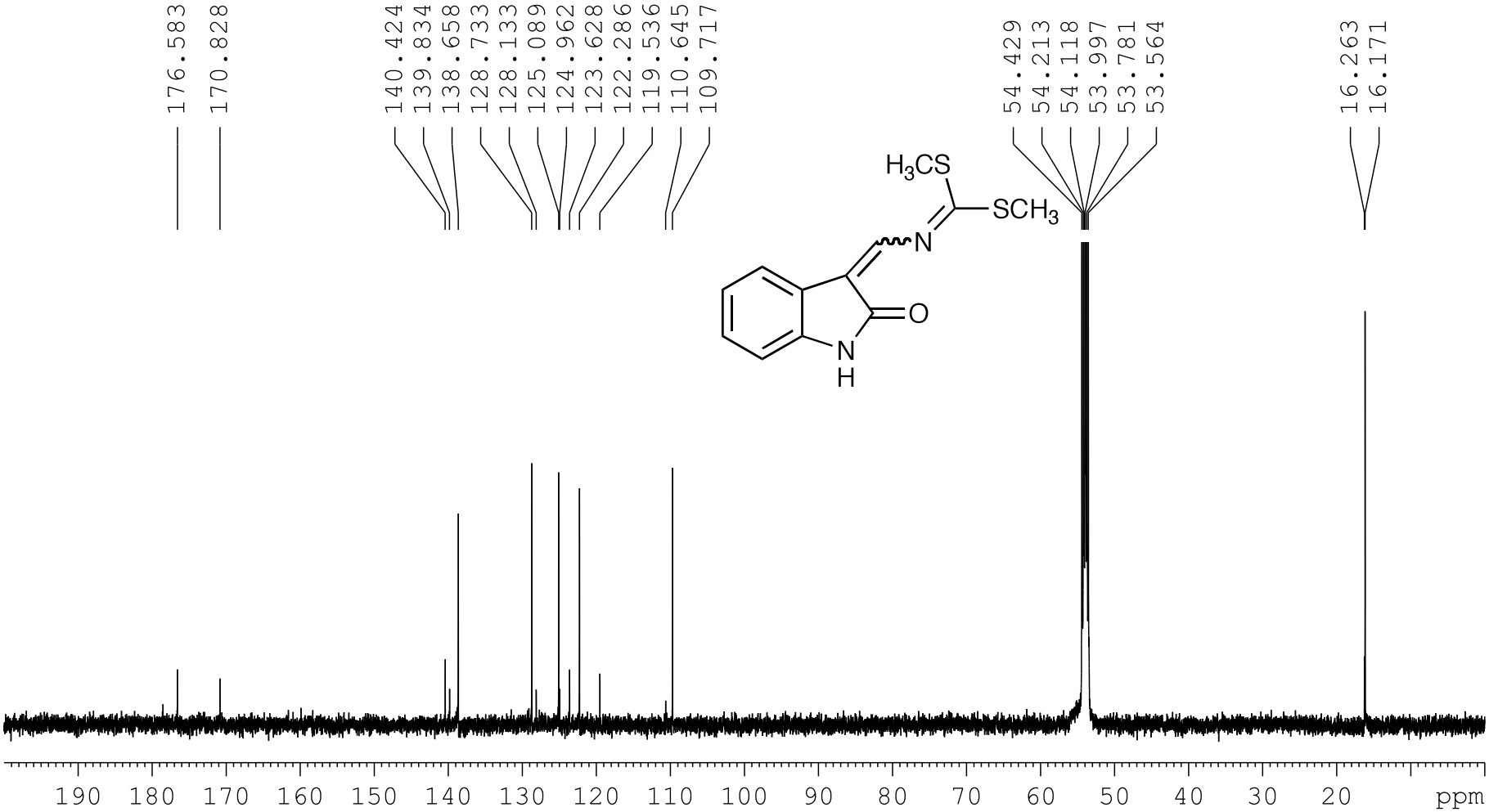
Demethoxydihydrowasalexin – ^{13}C NMR (CD_2Cl_2)



Demethoxywasalexins A and B - ^{1}H NMR (CD_2Cl_2)



Demethoxywasalexins A and B - ^{1}H NMR (CD_2Cl_2)



Demethoxywasalexins A and B – ^{13}C NMR