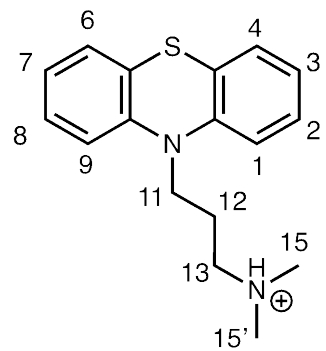


Structure-Binding Relationship of Permethylyated Cyclodextrins and Phenothiazine Drugs

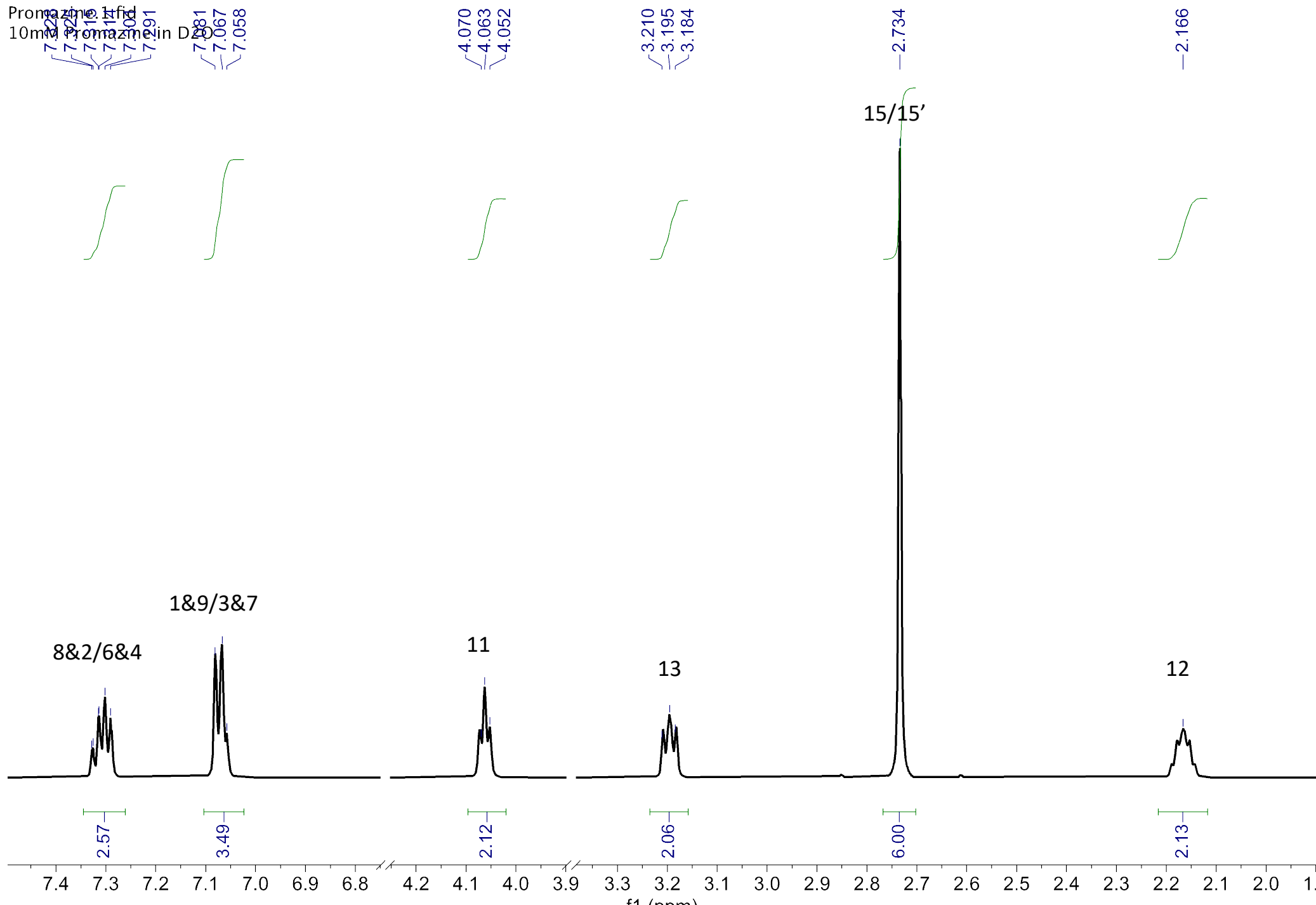
Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, 9500 Gilman Drive, La Jolla, California 92093-0751, USA

*mgilson@health.ucsd.edu

^1H NMR of Phenothiazine Compounds

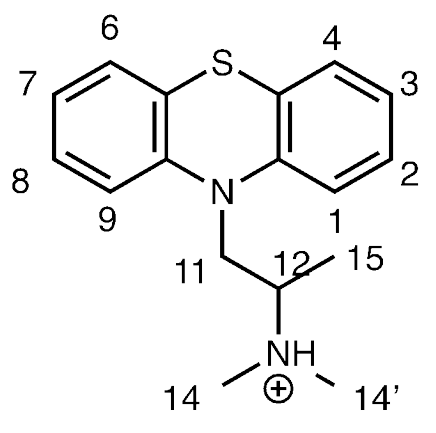


PMZ

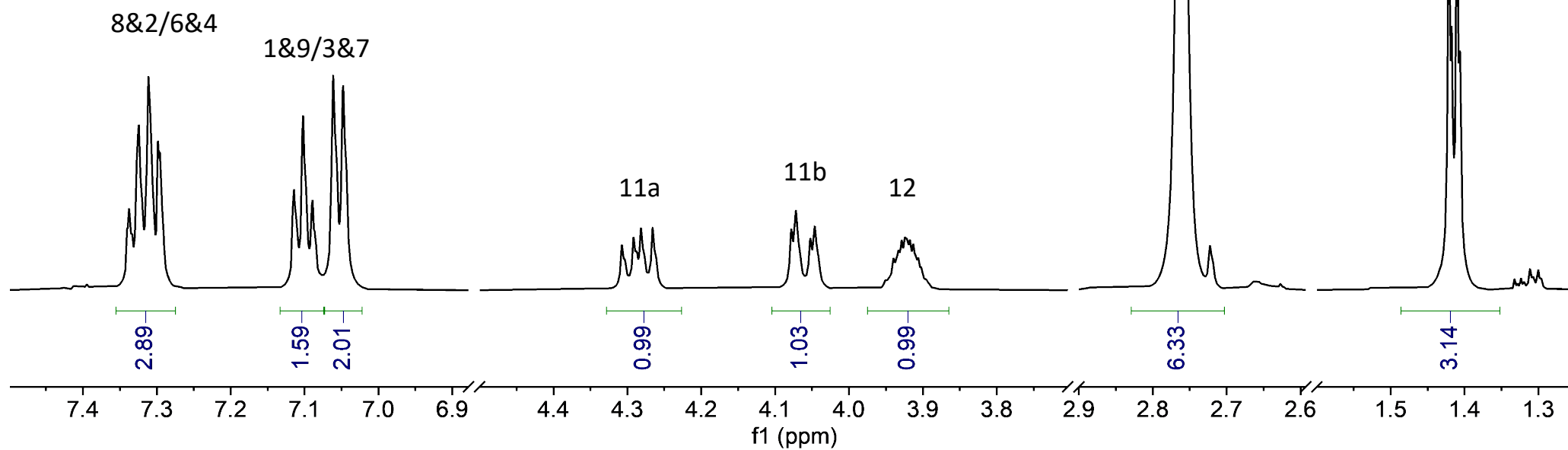


promethazine-1.fid
10mM Promethazine in D2O

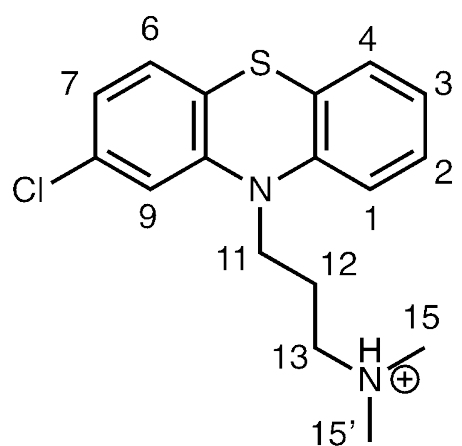
7.396
7.391
7.386
7.381
7.114
7.101
7.089
7.061
7.049
4.308
4.292
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4.266
4.072
4.046
3.922
2.756
1.422
1.417
1.410
1.406



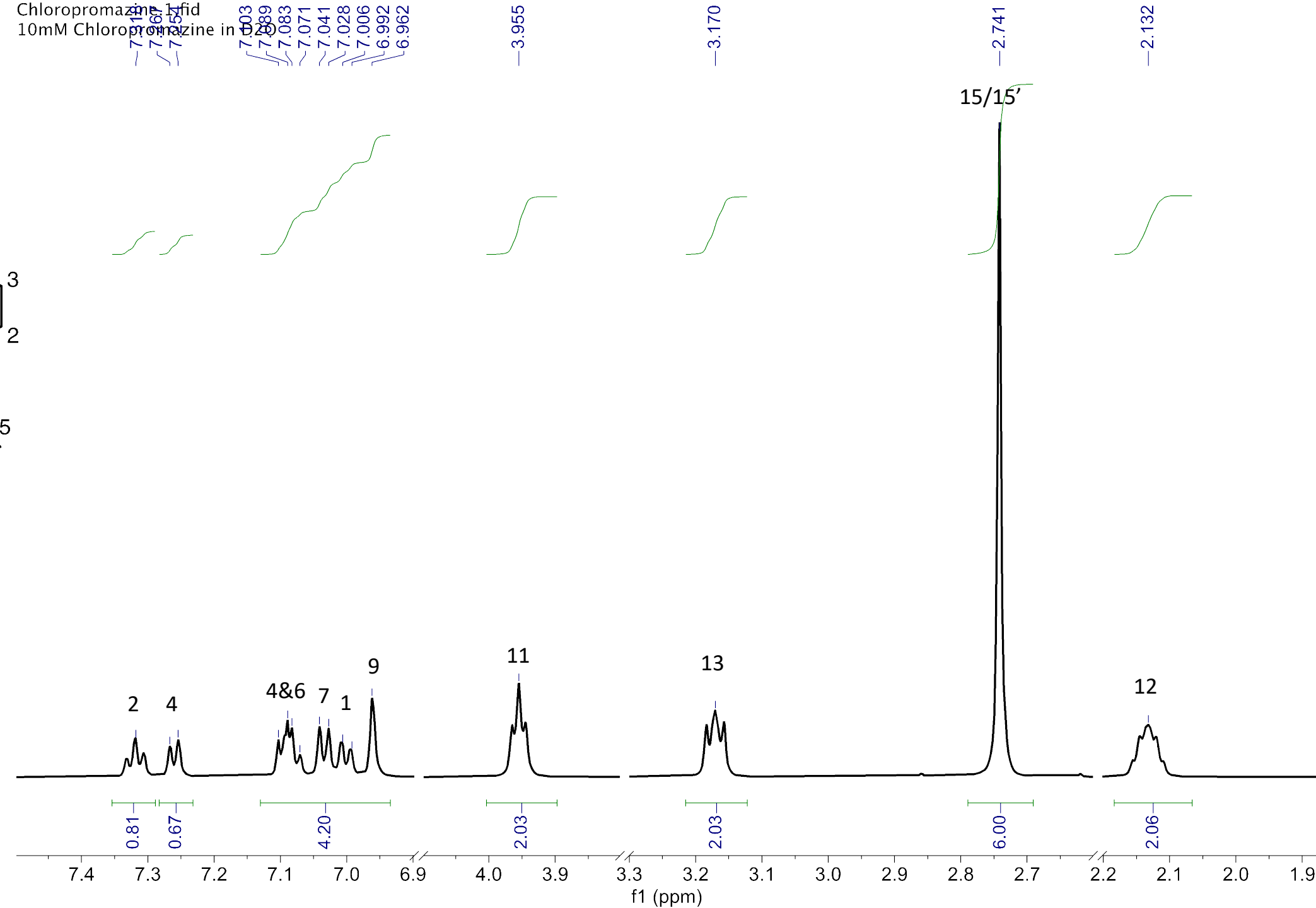
PMT

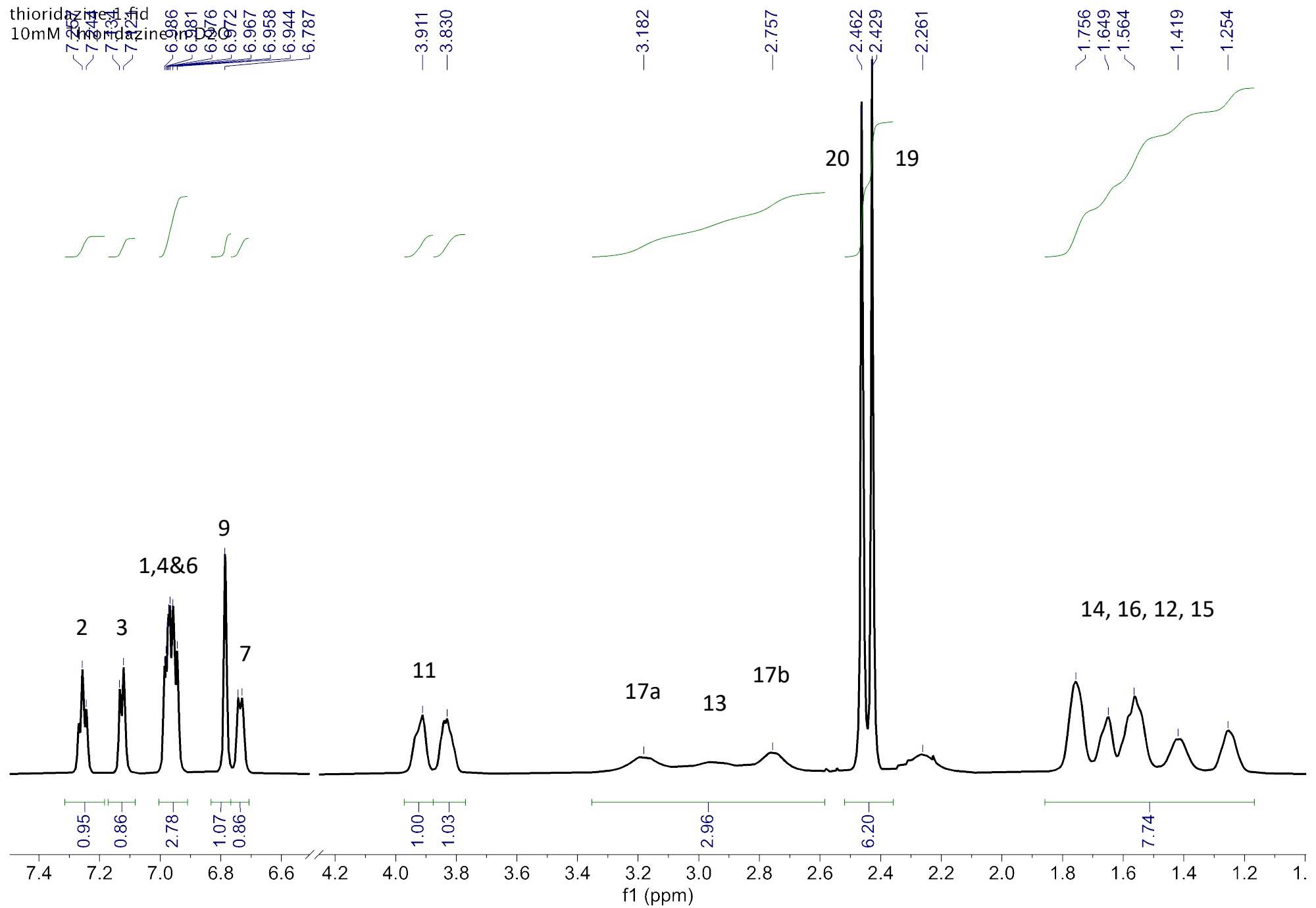
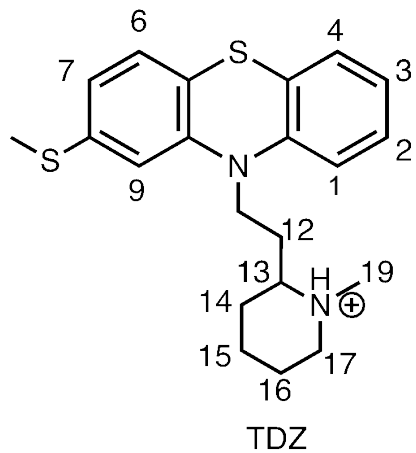


Chlorpromazine d₅-¹⁵DFD
10mM Chlorpromazine in D₂O

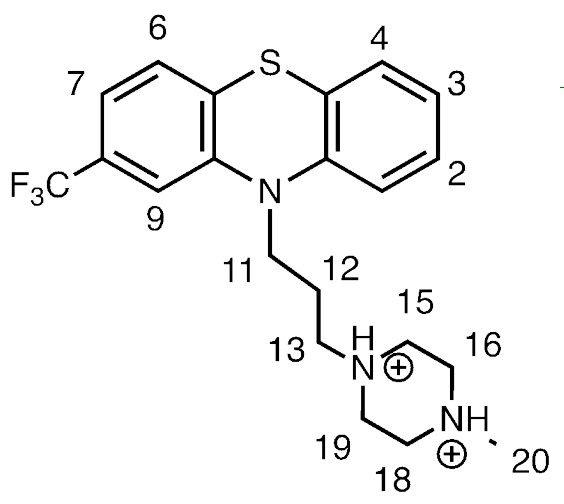


CPZ

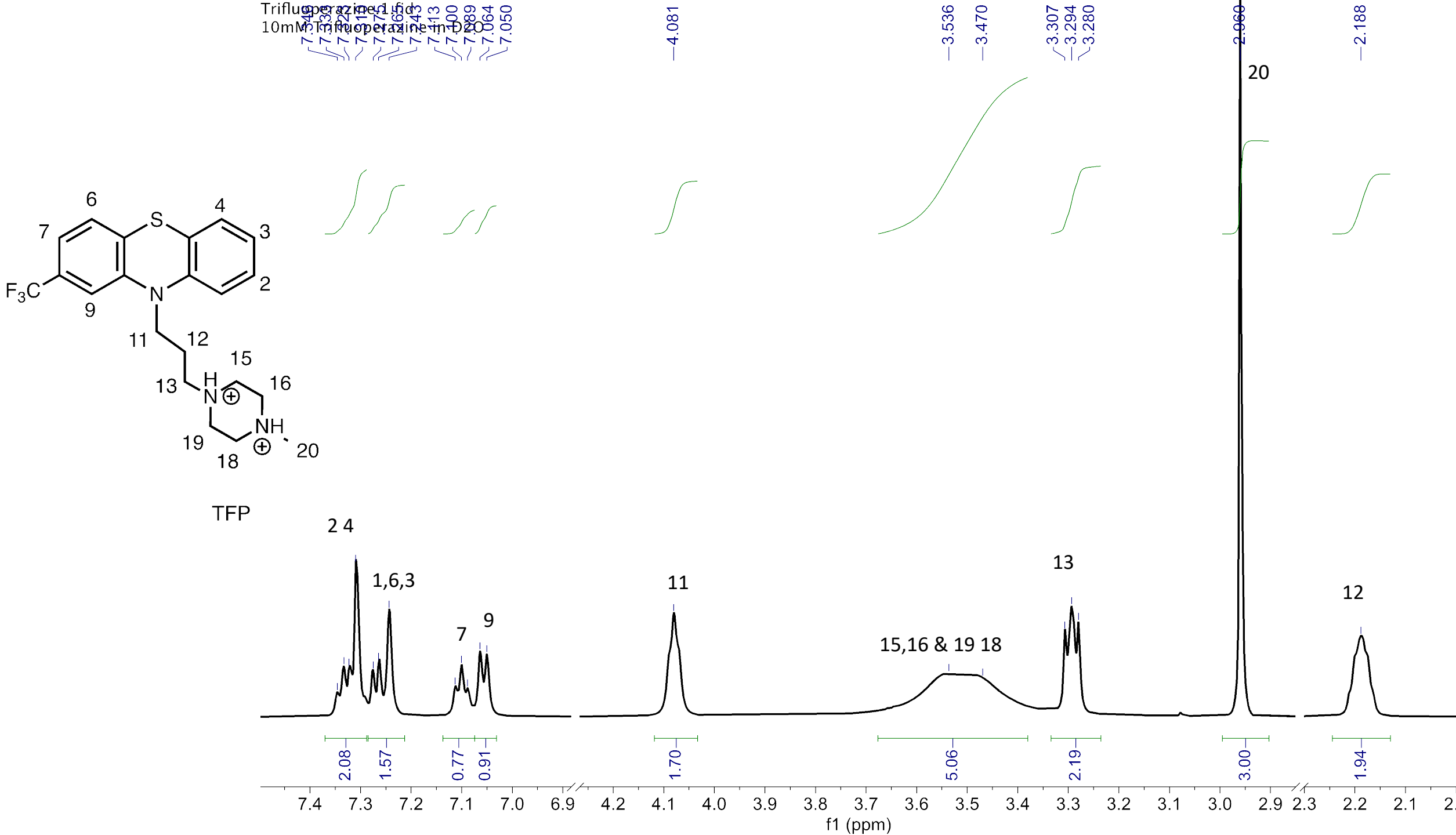
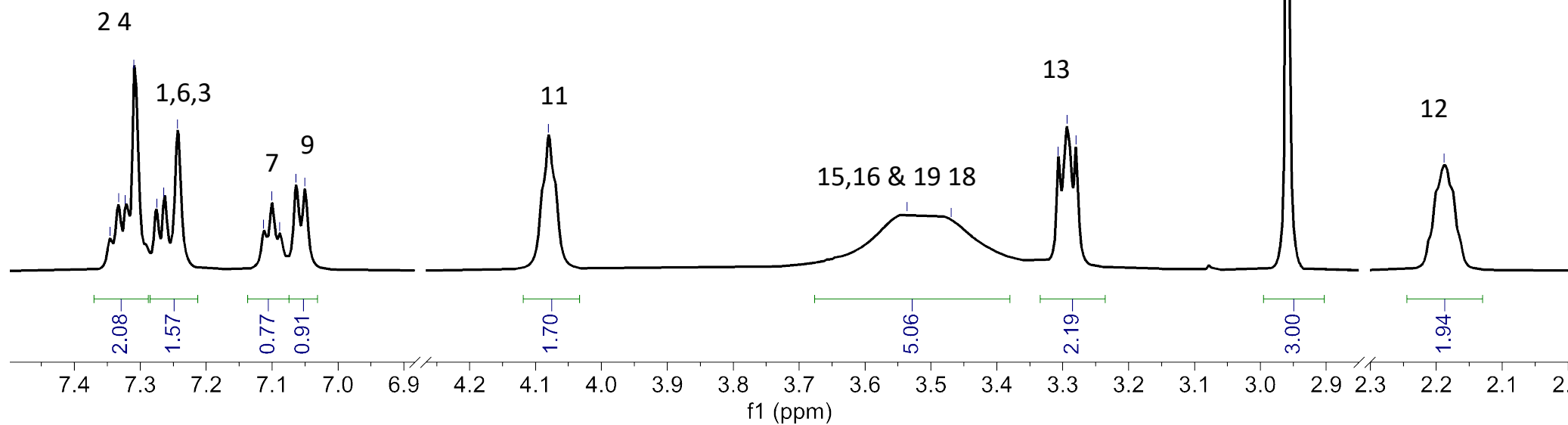




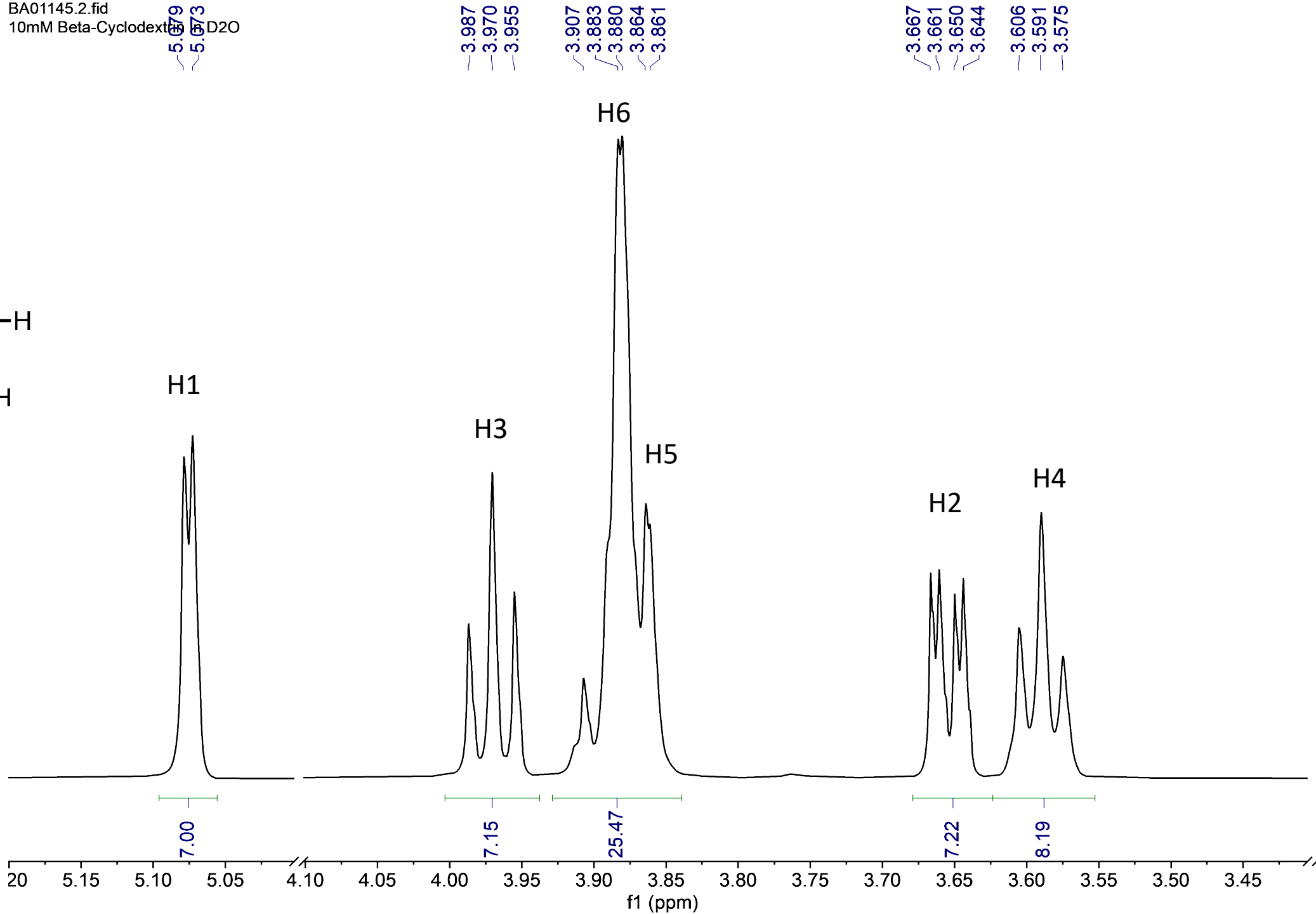
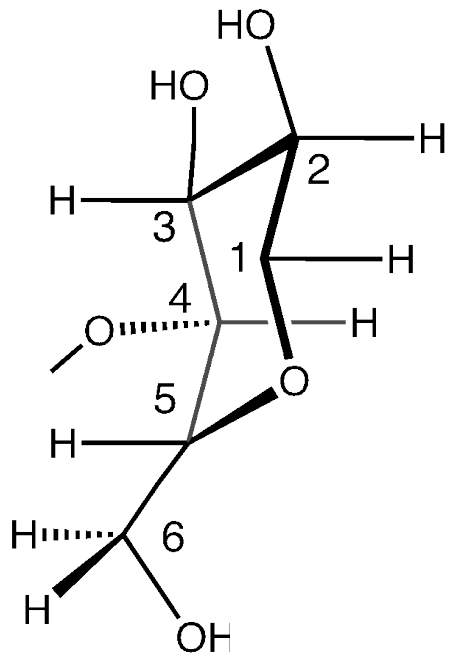
Trifluoperazine d₁ f1
10mM Trifluoperazine in D₂O



TFP



^1H NMR of Cyclodextrin Derivatives



O-6M-BCD.1.fid
Heptakis-(6-O-methyl)- β -CD 10mM

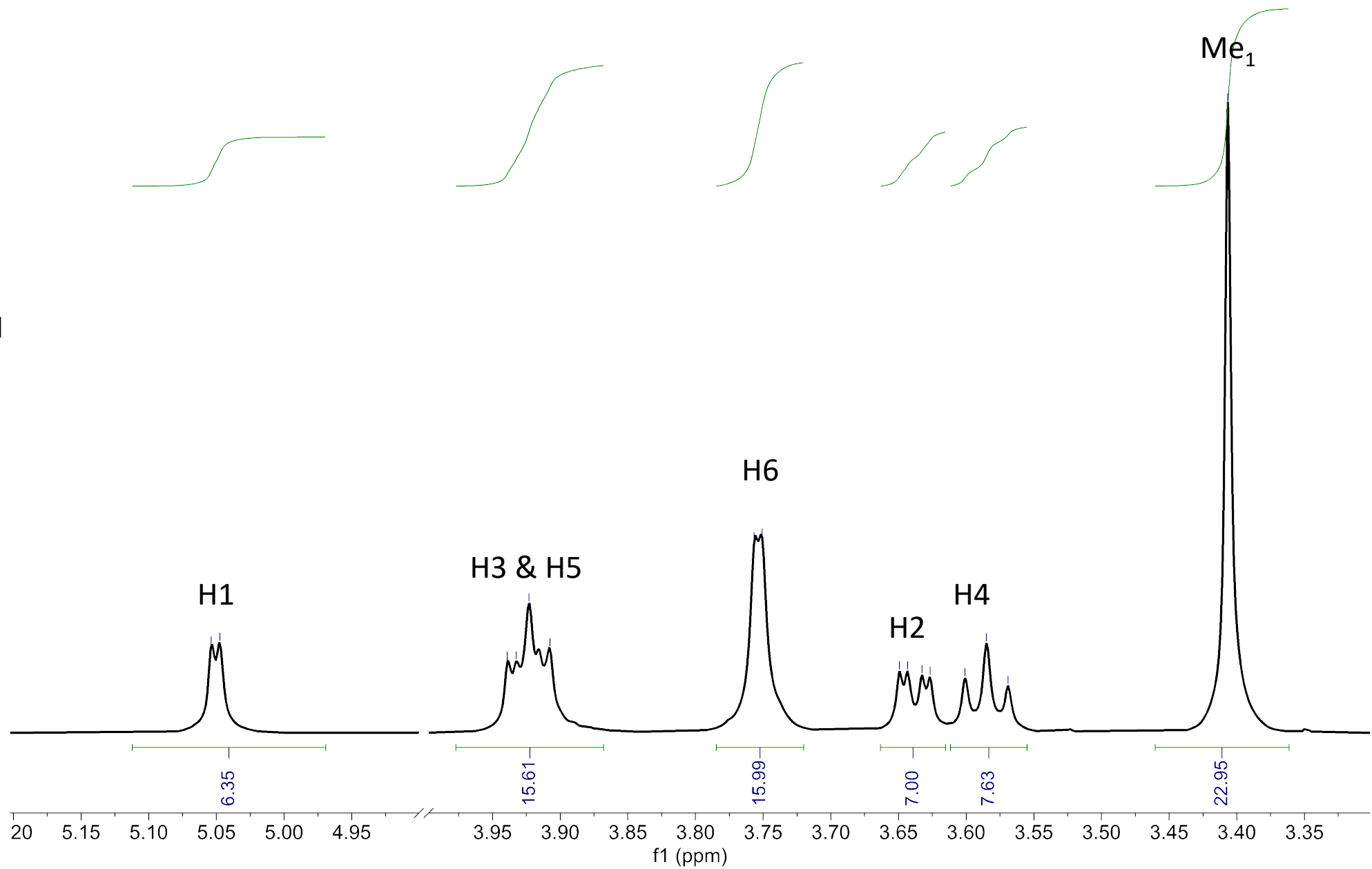
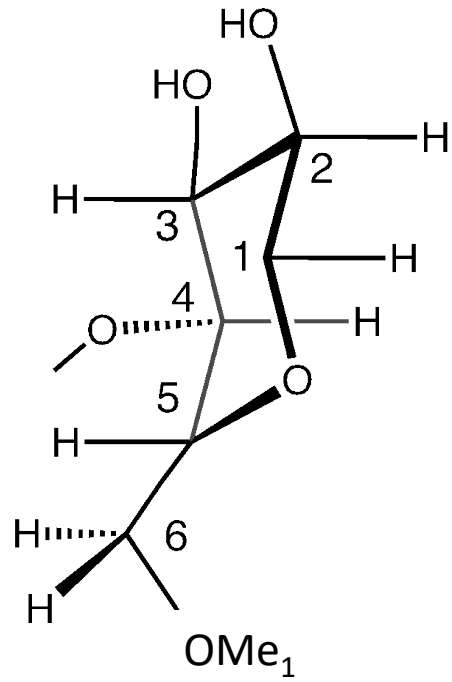
5.054
5.047

3.939
3.932
3.923
3.907

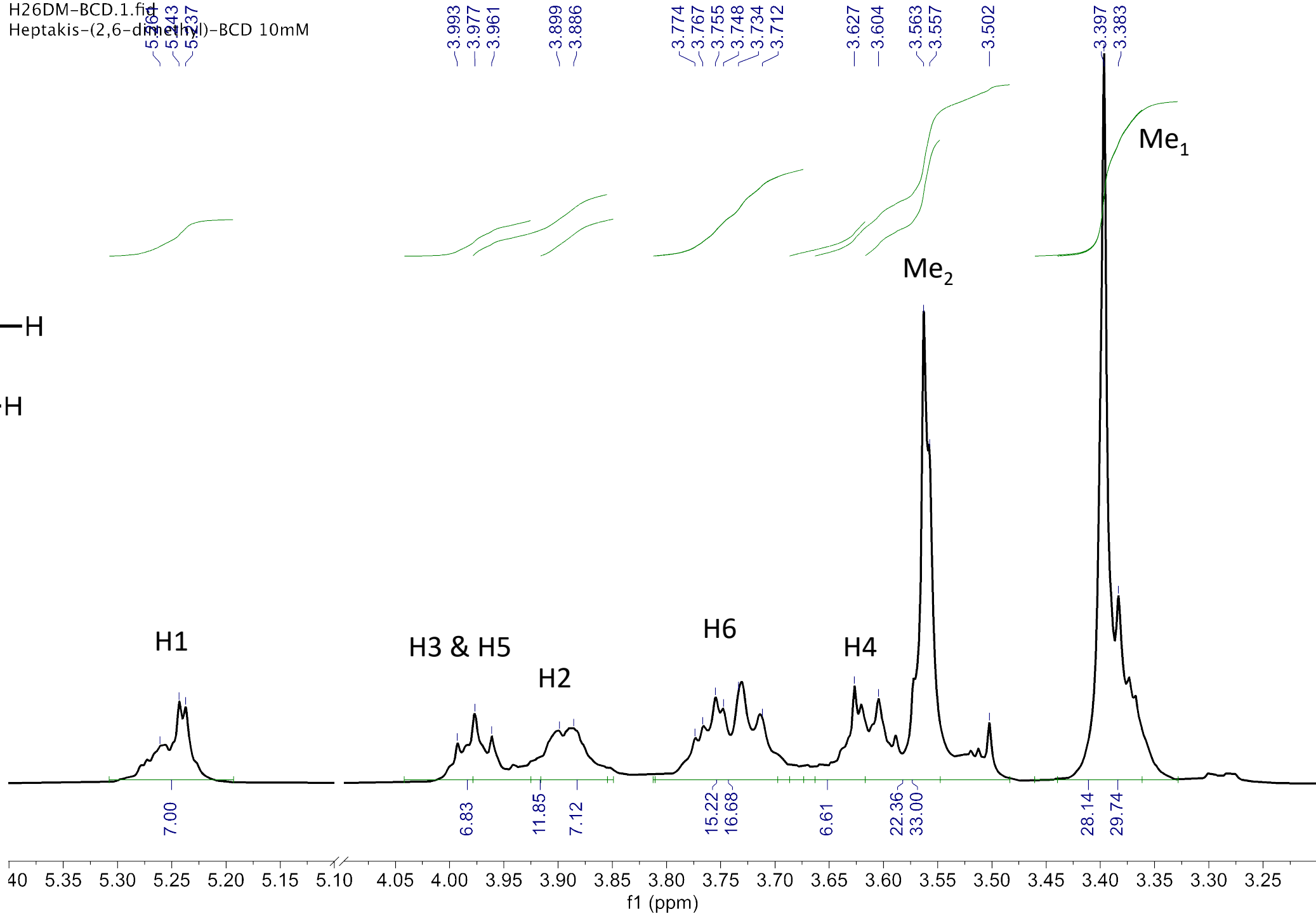
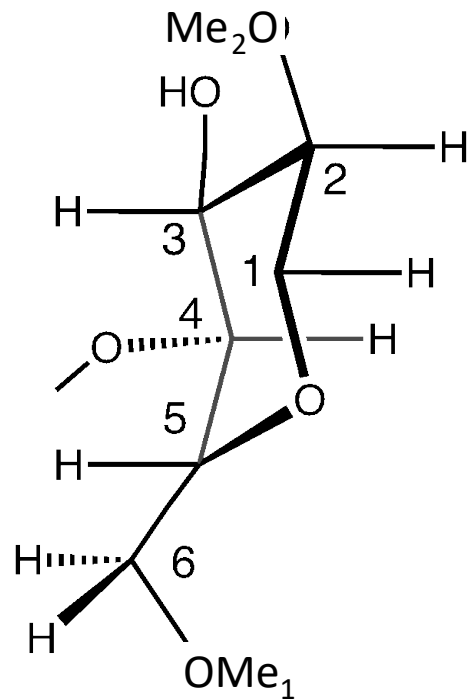
3.757
3.751

3.649
3.643
3.633
3.627
3.601
3.585
3.569

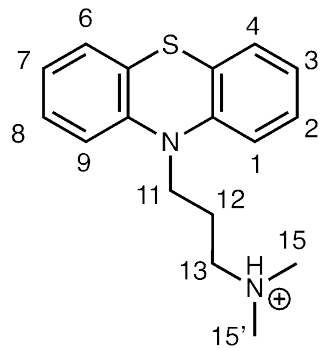
3.407



H26DM-BCD.1.fid
Heptakis-(2,6-dimethyl)-BCD 10mM

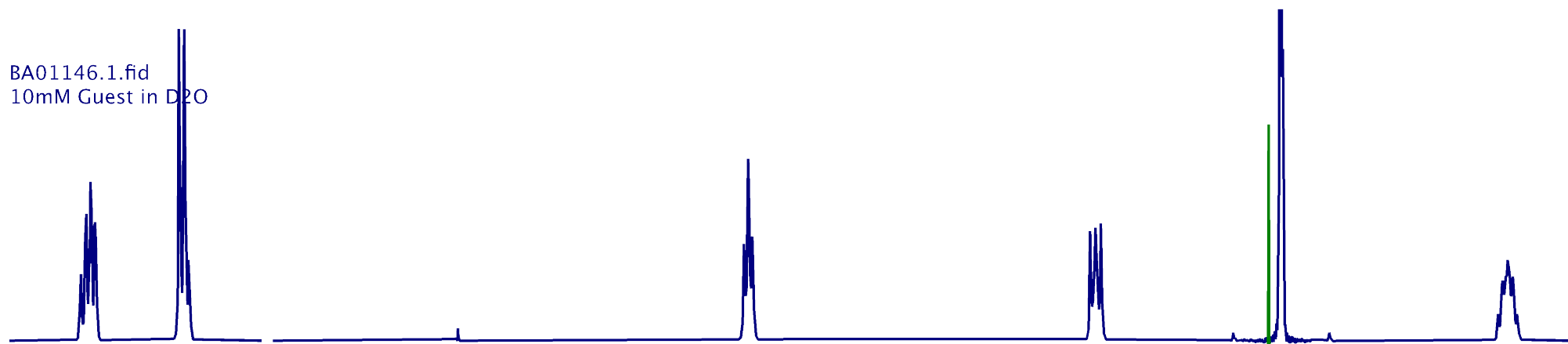


^1H NMR of β -CD with Phenothiazines

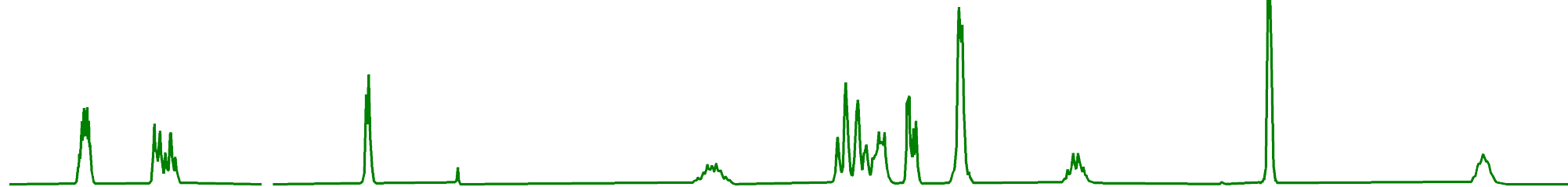


PMZ

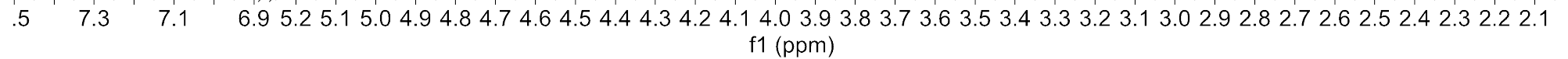
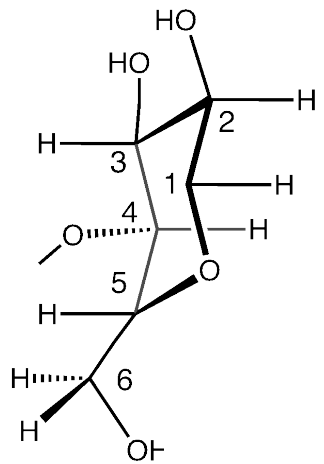
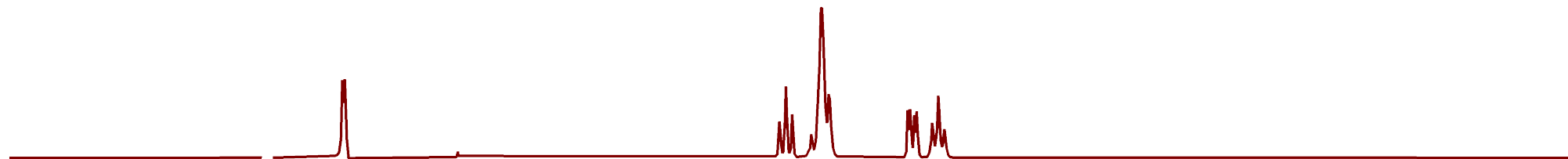
BA01146.1.fid
10mM Guest in D₂O

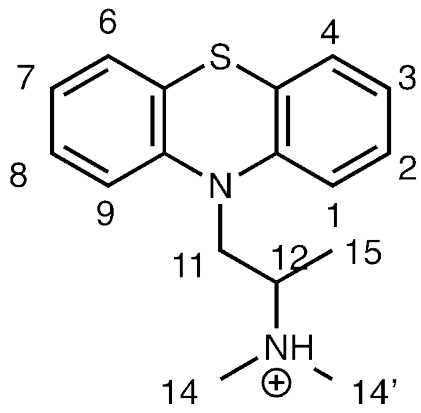


BA01146.2.fid
5mM 1:1 Complex in D₂O



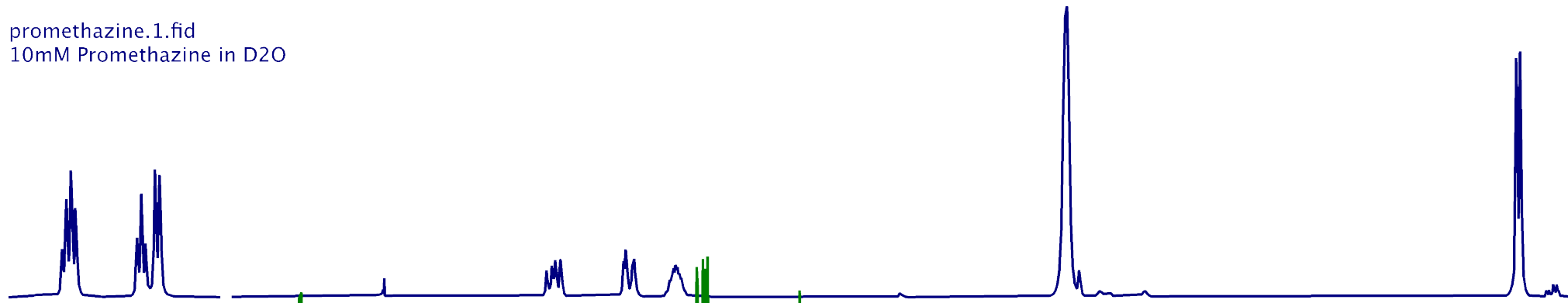
BA01145.2.fid
10mM Beta-Cyclodextrin in D₂O



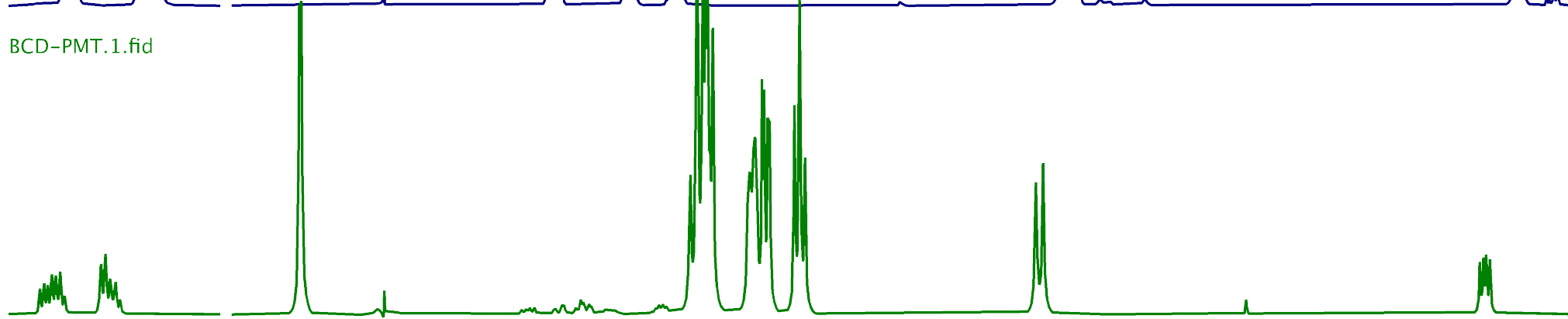


PMT

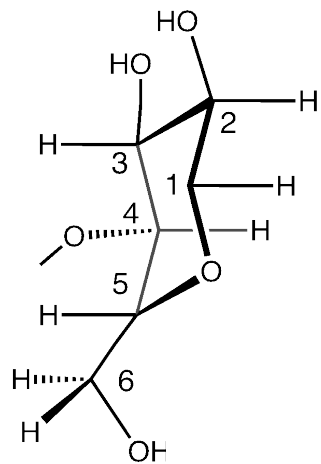
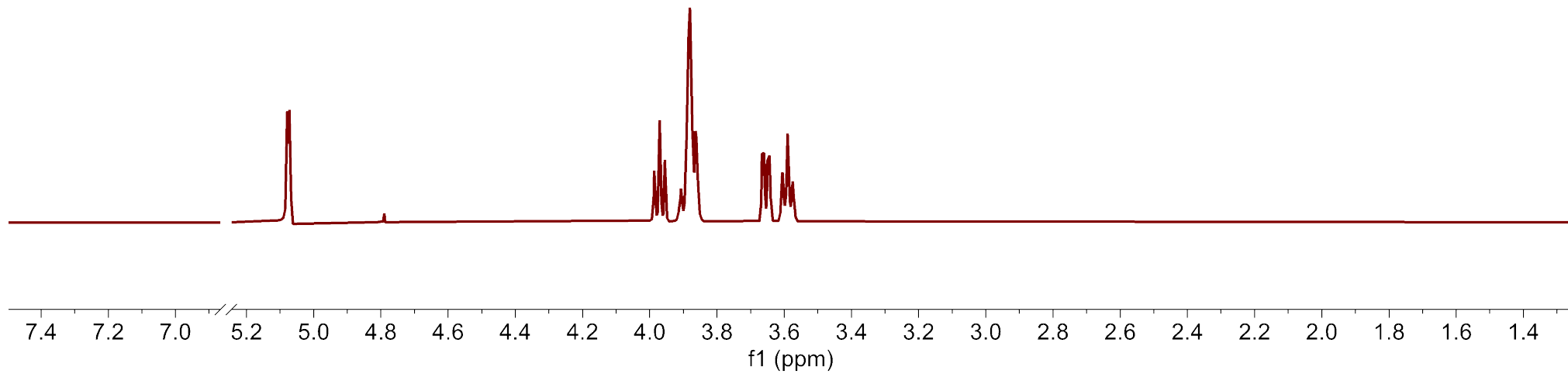
promethazine.1.fid
10mM Promethazine in D₂O

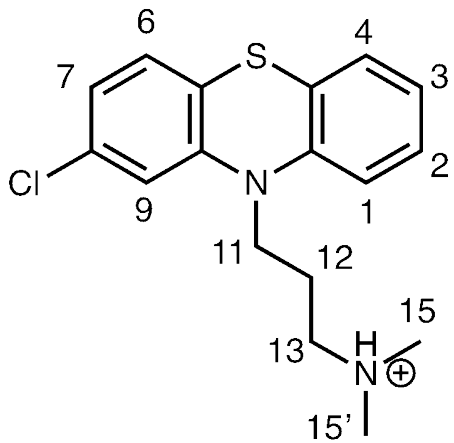


BCD-PMT.1.fid



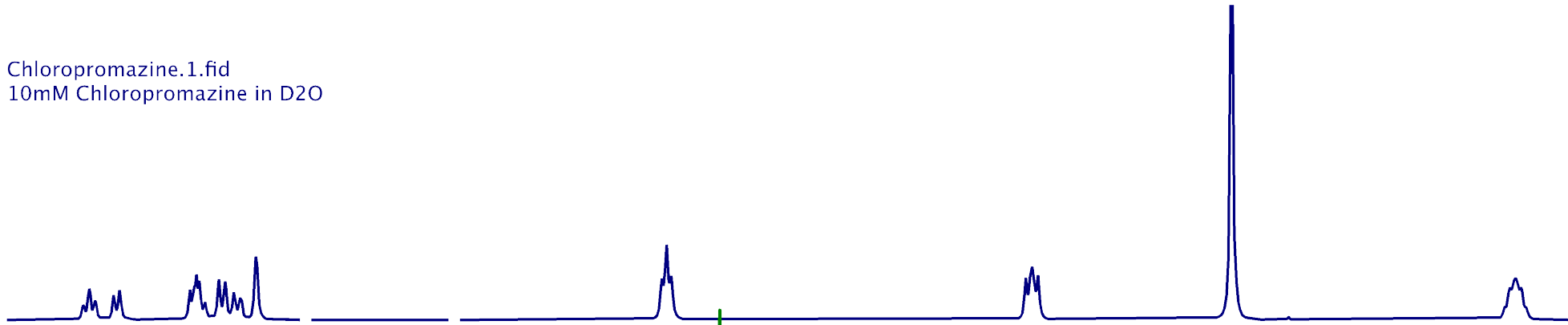
BA01145.2.fid
10mM Beta-Cyclodextrin in D₂O



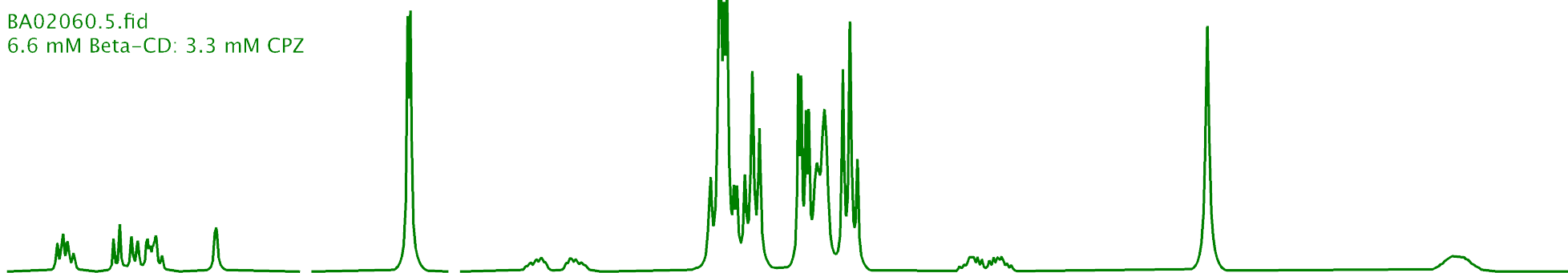


CPZ

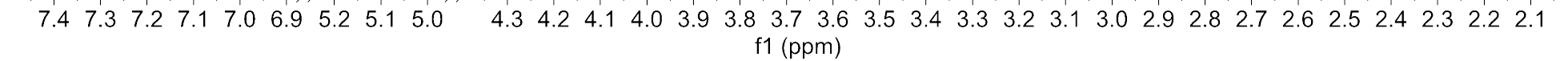
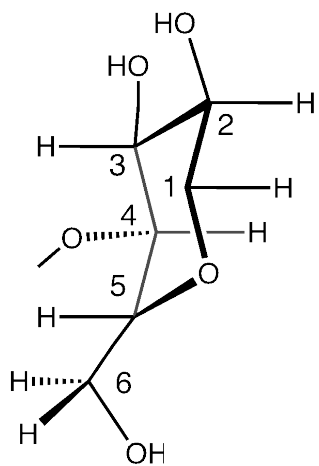
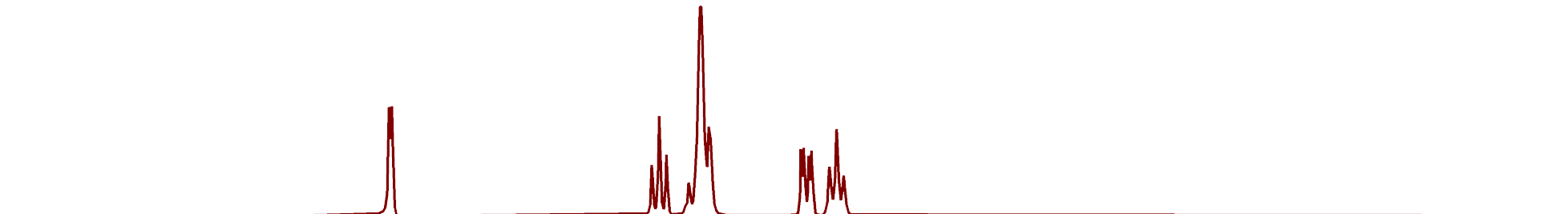
Chlorpromazine.1.fid
10mM Chlorpromazine in D2O

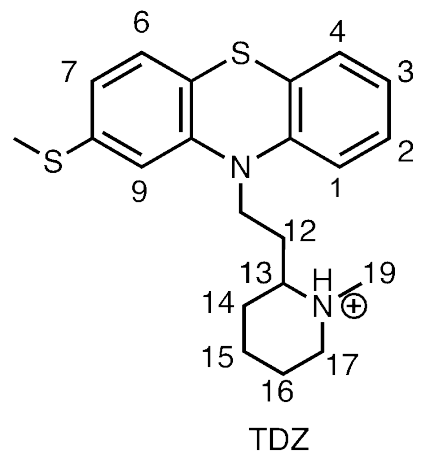


BA02060.5.fid
6.6 mM Beta-CD: 3.3 mM CPZ

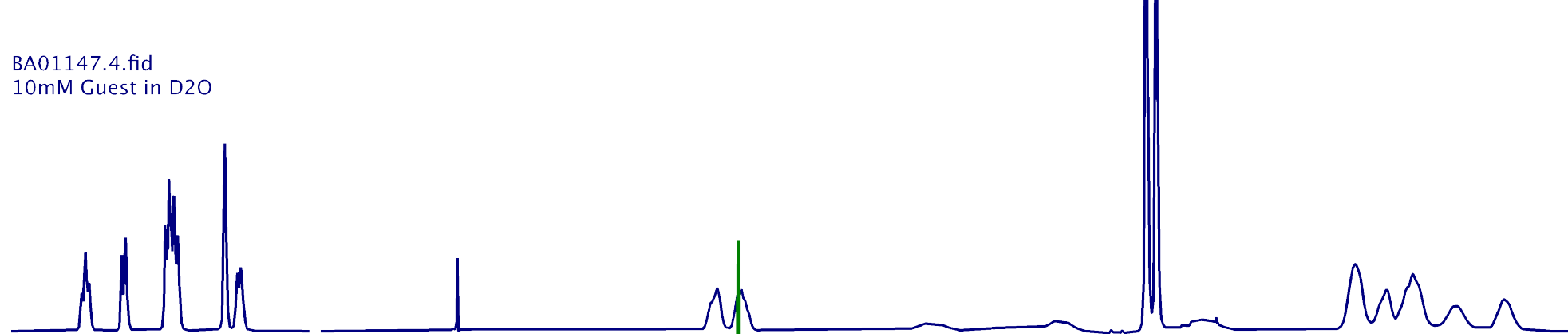


BA01145.2.fid
10mM Beta-Cyclodextrin in D2O

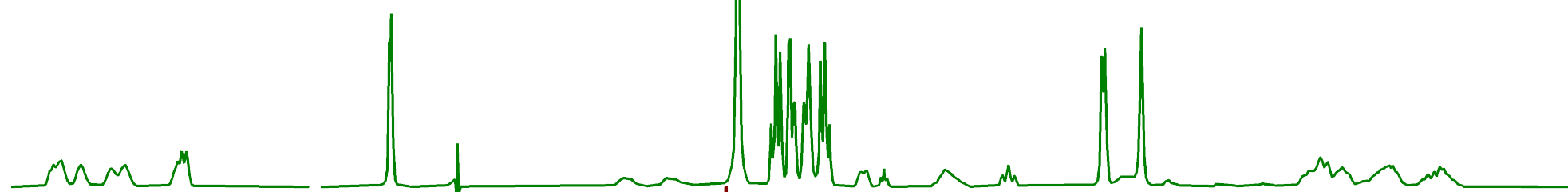




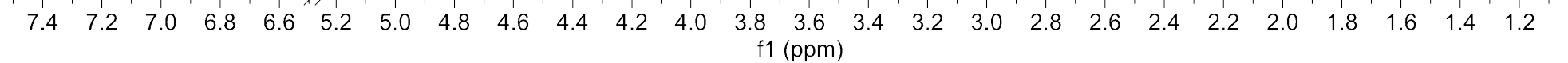
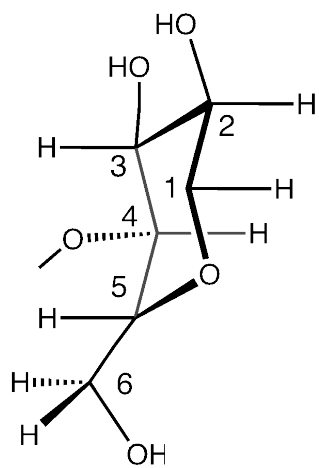
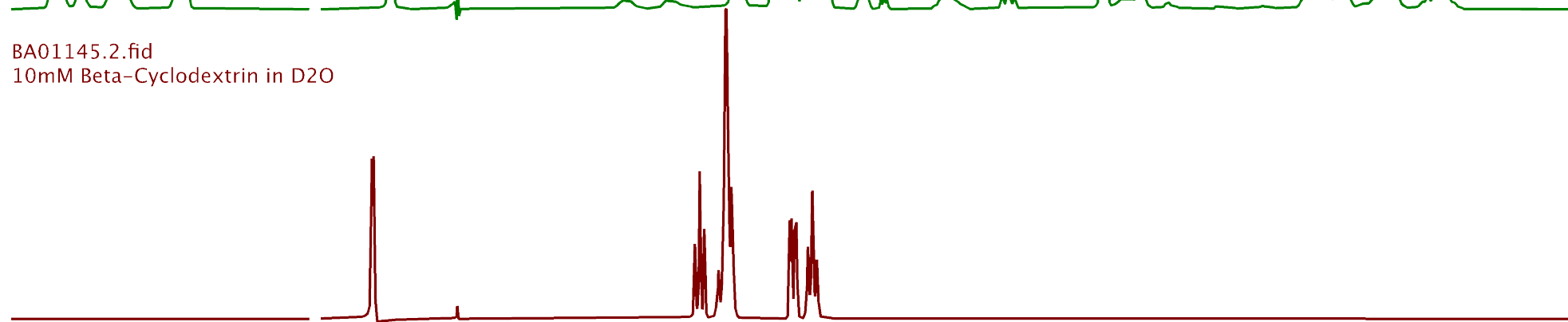
BA01147.4.fid
10mM Guest in D2O

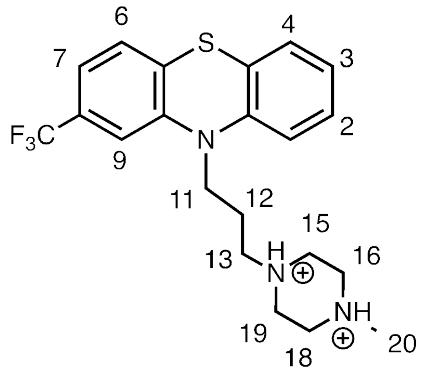


BA01147.2.fid
5mM 1:1 Complex in D2O



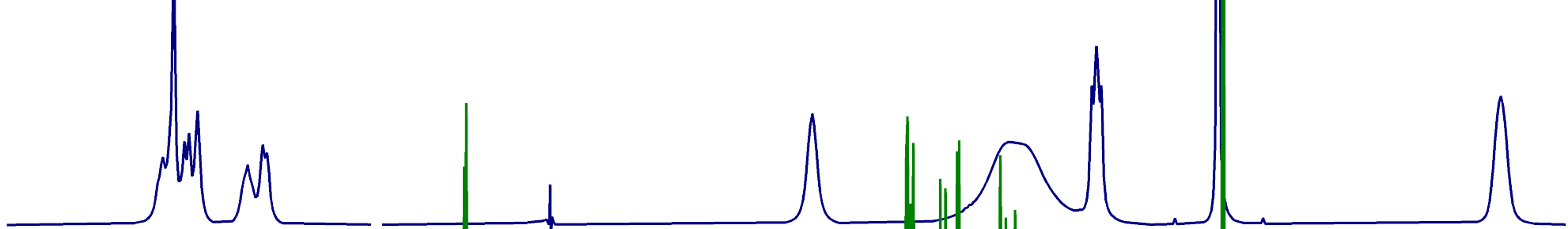
BA01145.2.fid
10mM Beta-Cyclodextrin in D2O



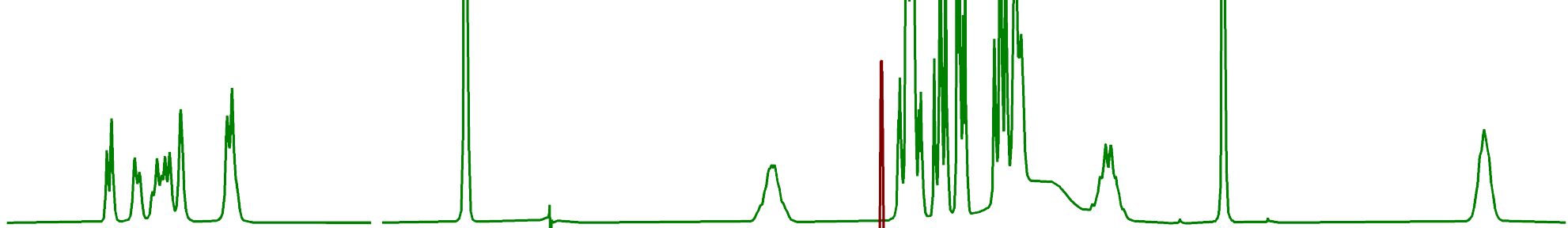


TFP

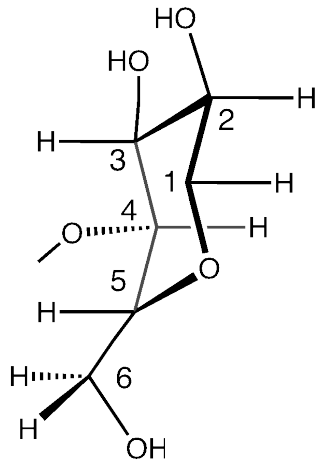
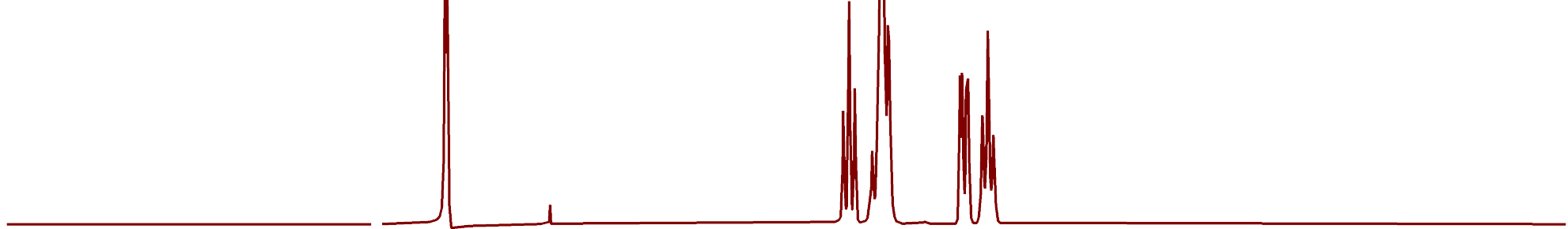
BA01148.1.fid
10mM Guest in D₂O



BA01148.2.fid
5mM 1:1 Complex in D₂O



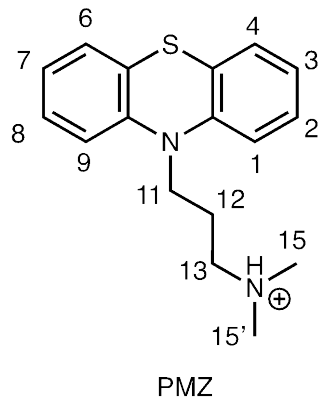
BA01145.2.fid
10mM Beta-Cyclodextrin in D₂O



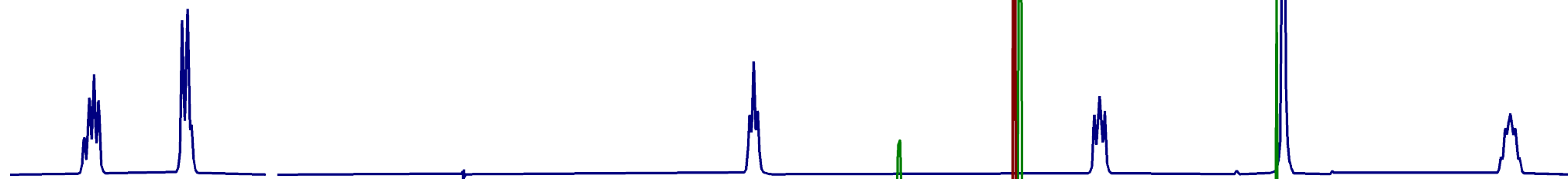
7.6 7.4 7.2 7.0 6.8 // 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2

f1 (ppm)

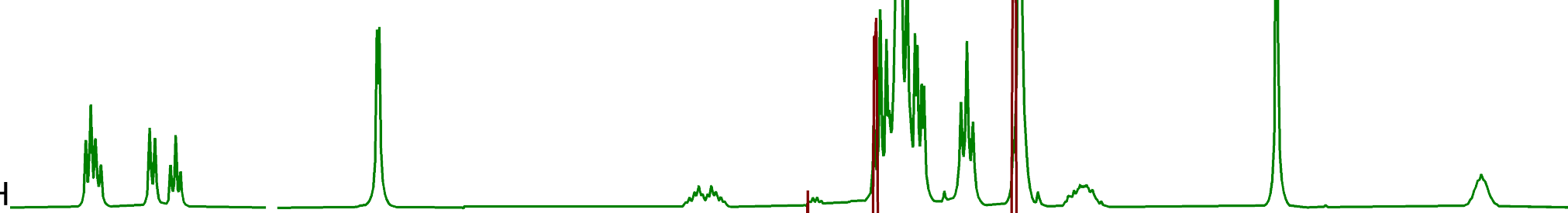
^1H NMR of MM- β -CD
with Phenothiazines



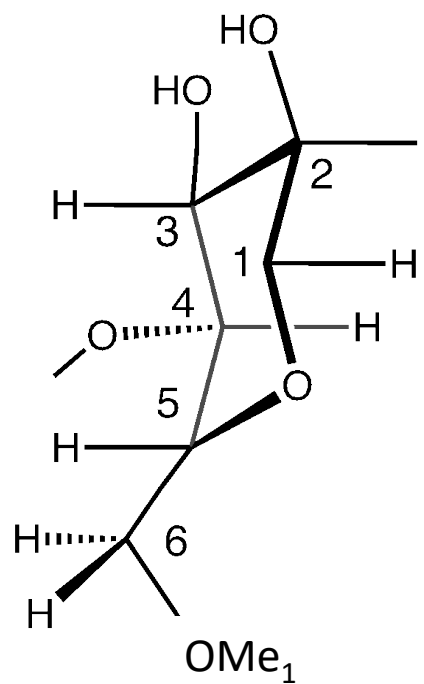
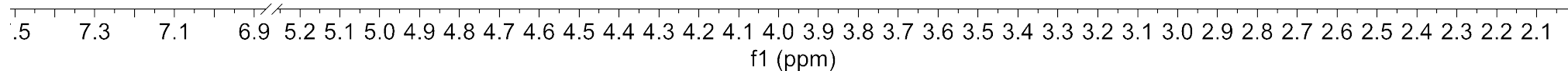
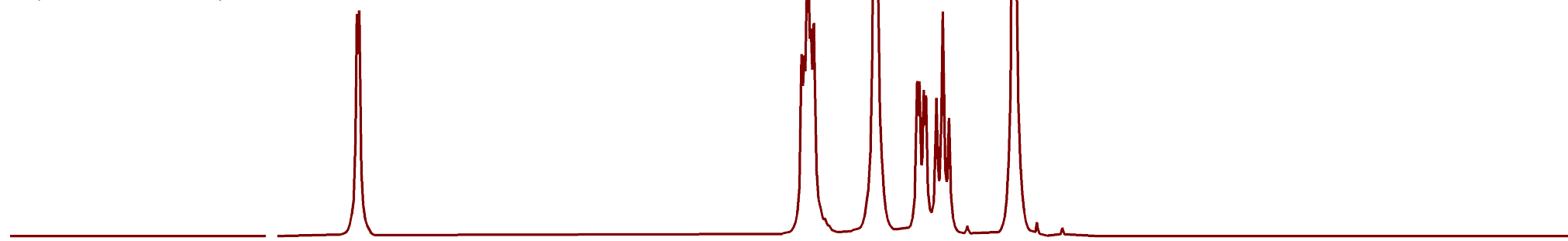
Promazine.1.fid
10mM Promazine in D2O

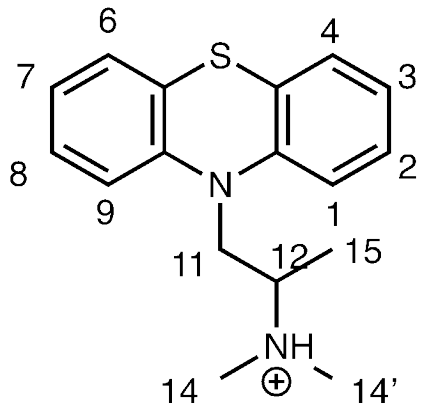


O-6Me-BCD-Phenothiazine.1.fid
O-6Me-BCD:PMZ 6mM:4mM

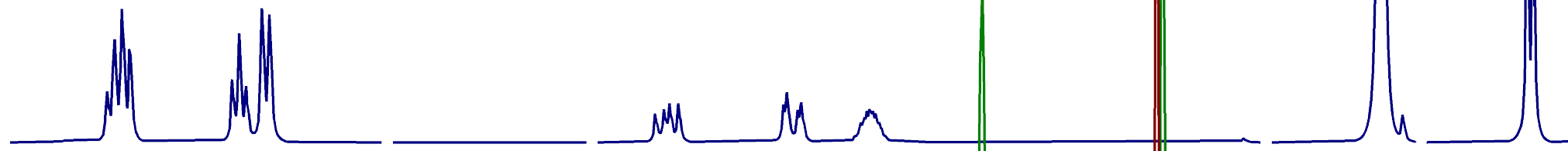


O-6M-BCD.1.fid
Heptakis-(6-O-methyl)-BCD 10mM



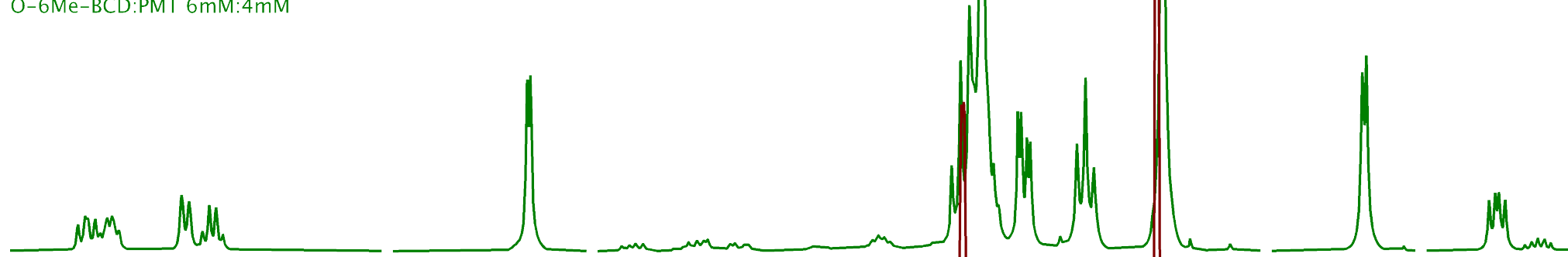


promethazine.1.fid
10mM Promethazine in D2O

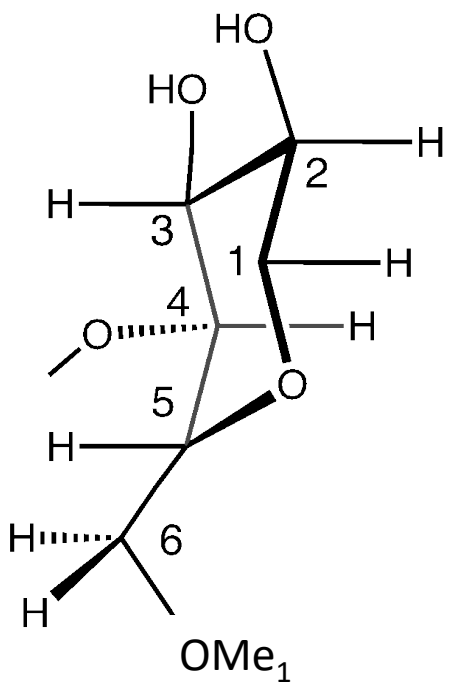
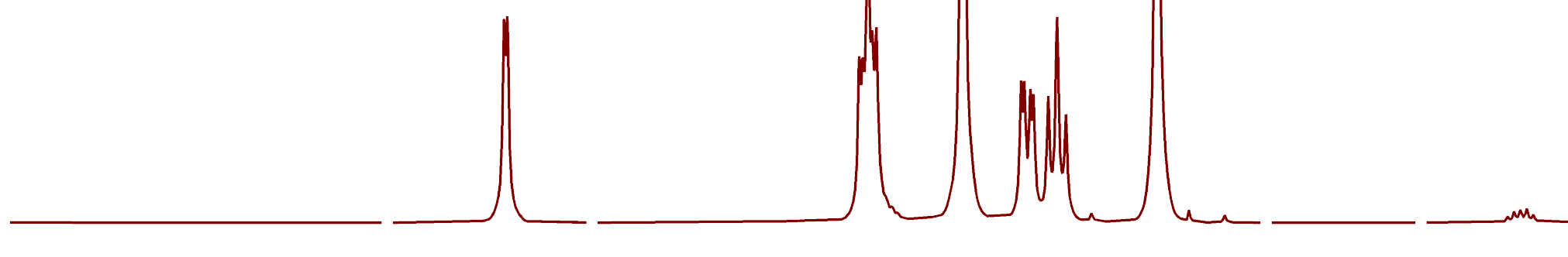


O-6Me-BCD-Phenothiazine.3.fid
O-6Me-BCD:PMT 6mM:4mM

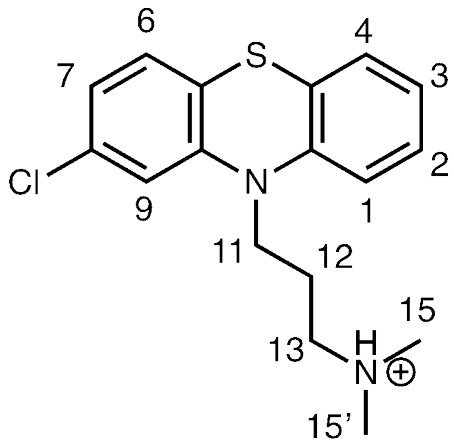
PMT



O-6M-BCD.1.fid
Heptakis-(6-O-methyl)-BCD 10mM

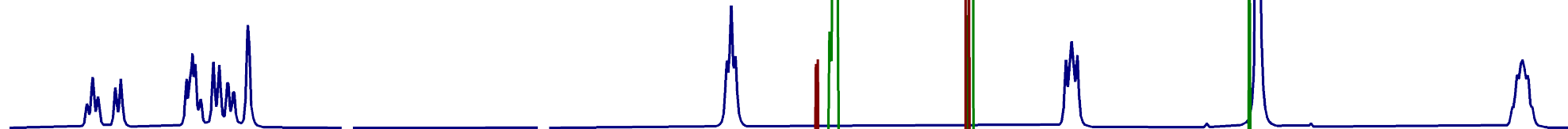


f1 (ppm)

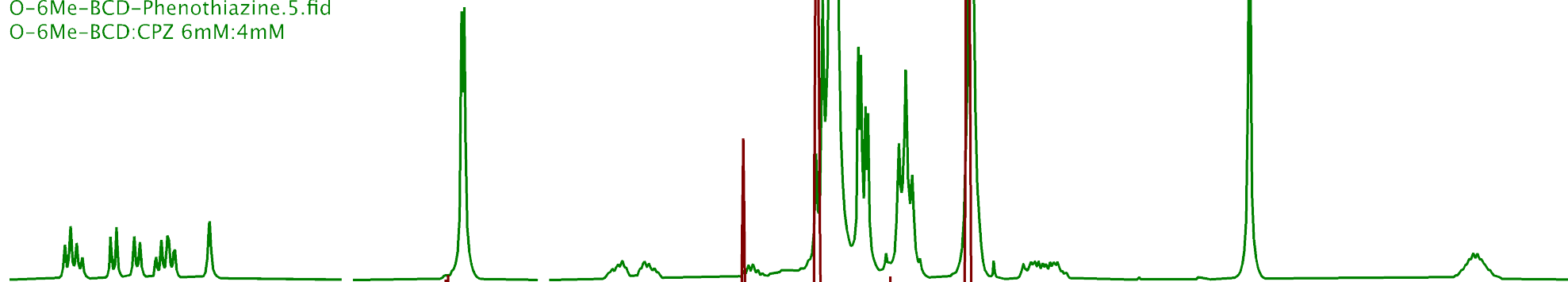


CPZ

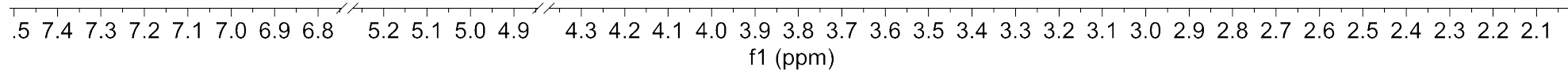
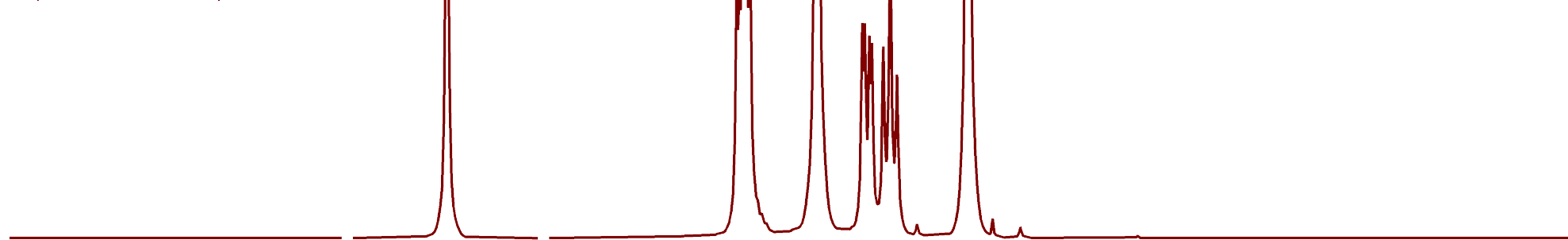
Chlorpromazine.1.fid
10mM Chlorpromazine in D2O



O-6Me-BCD-Phenothiazine.5.fid
O-6Me-BCD:CPZ 6mM:4mM

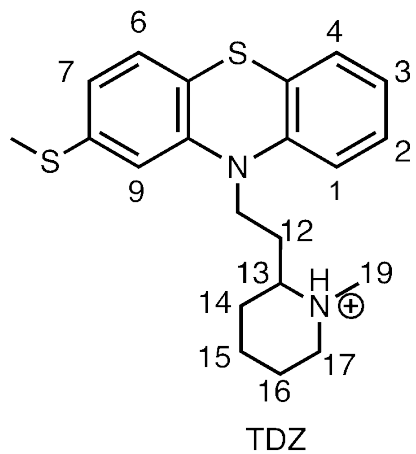


O-6M-BCD.1.fid
Heptakis-(6-O-methyl)-BCD 10mM

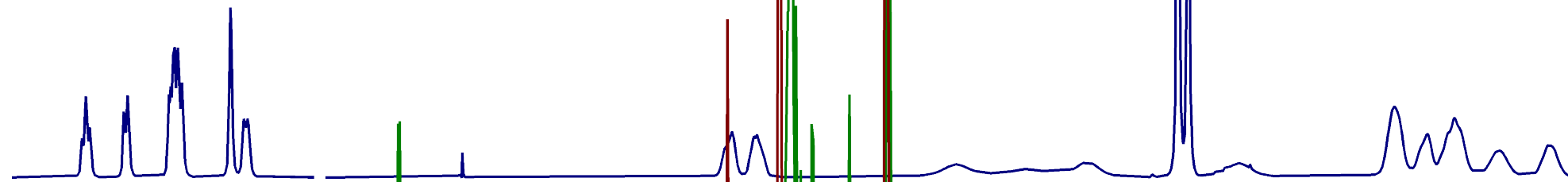


OMe₁

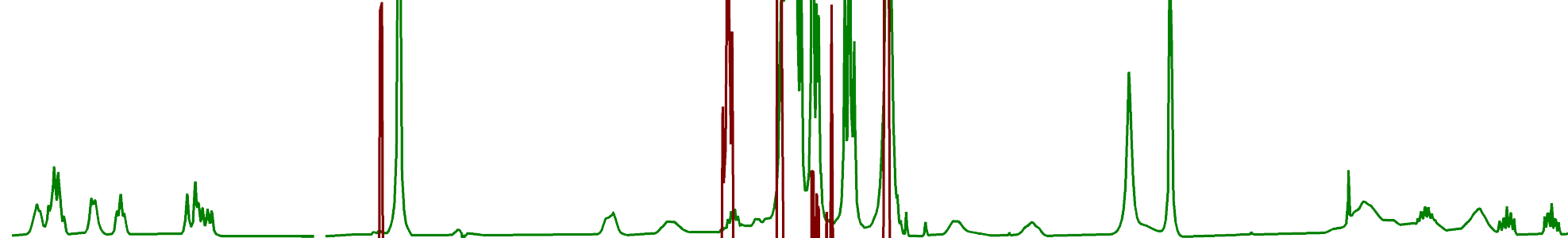
f1 (ppm)



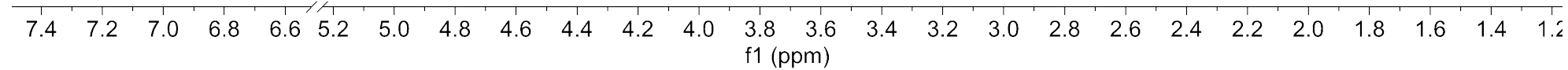
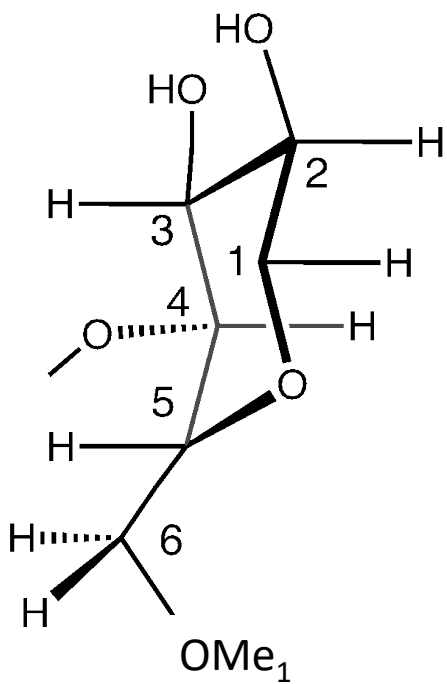
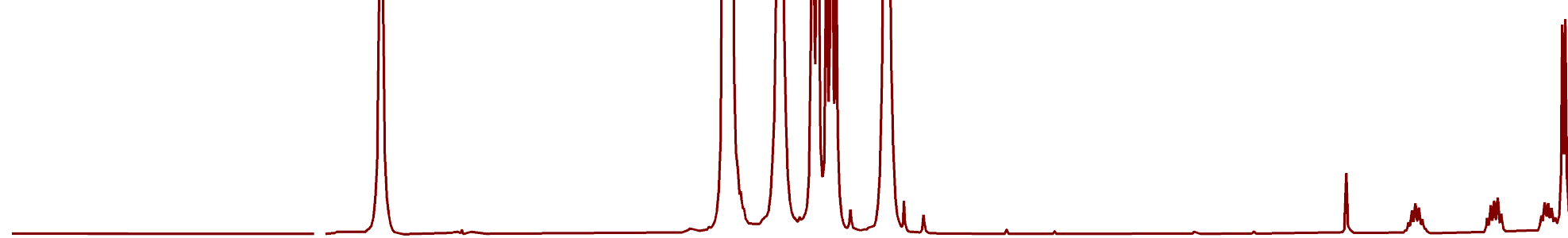
thioridazine.1.fid
10mM Thioridazine in D2O

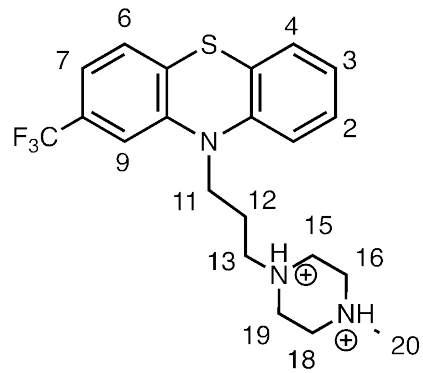


O-6Me-BCD-Phenothiazine.7.fid
O-6Me-BCD: TDZ 6mM:4mM



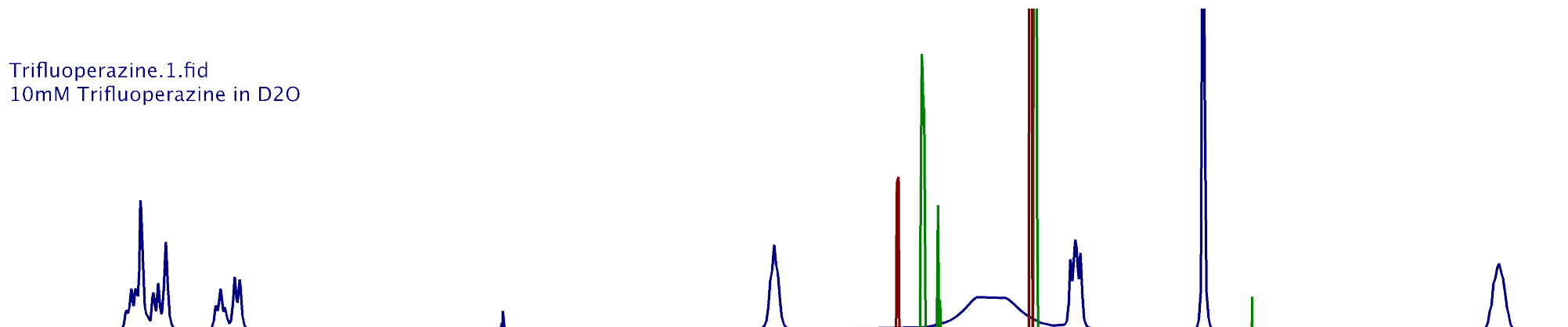
O-6M-BCD.1.fid
Heptakis-(6-O-methyl)-BCD 10mM



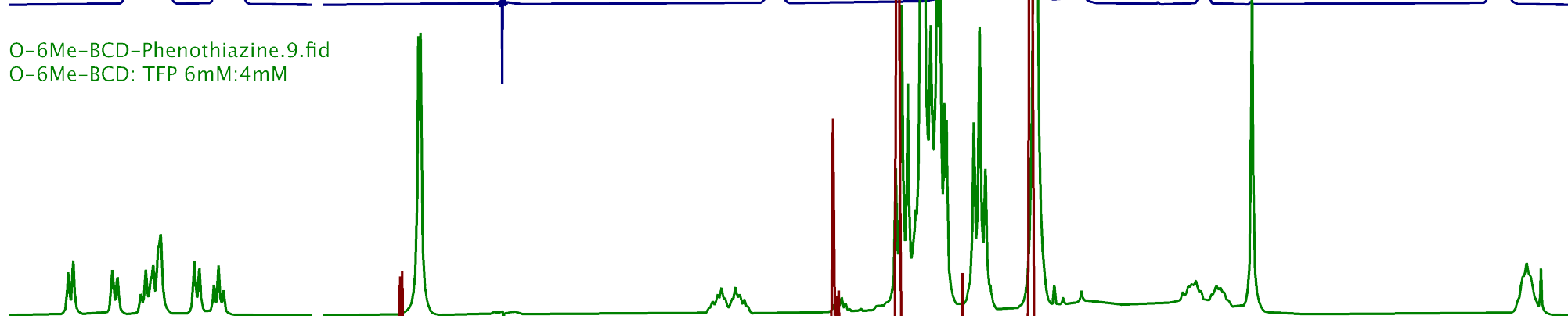


TFP

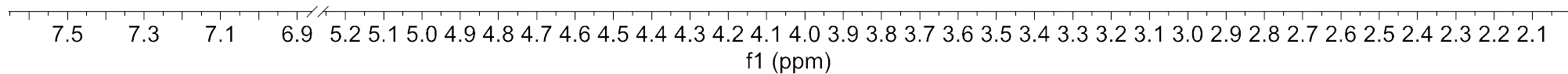
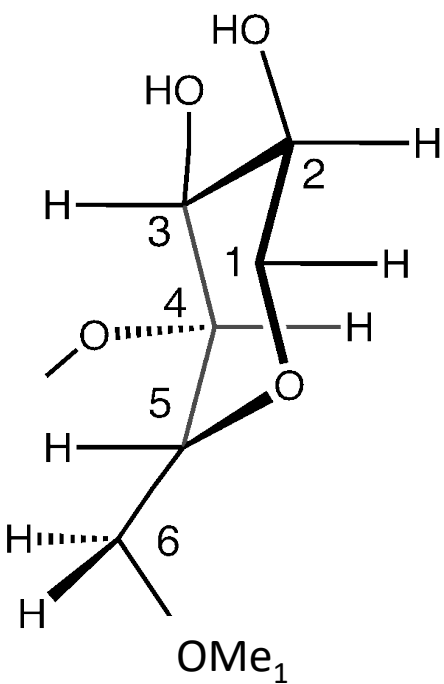
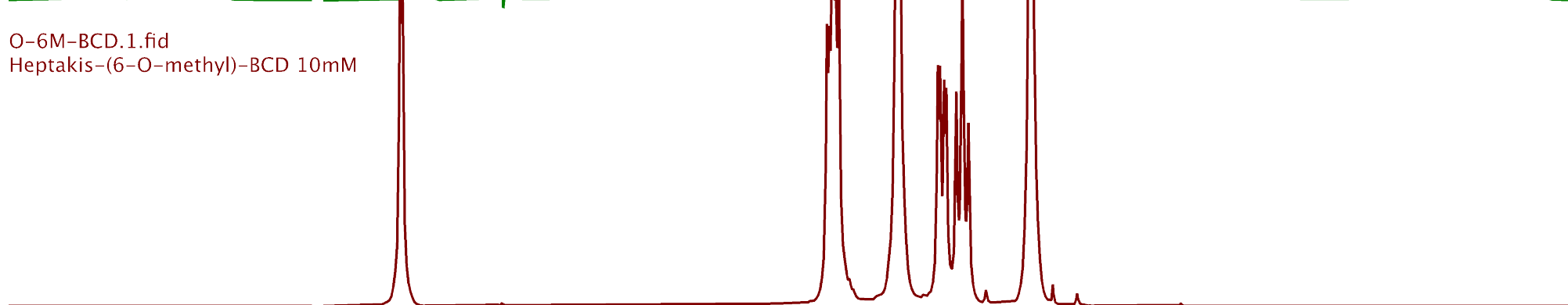
Trifluoperazine.1.fid
10mM Trifluoperazine in D2O



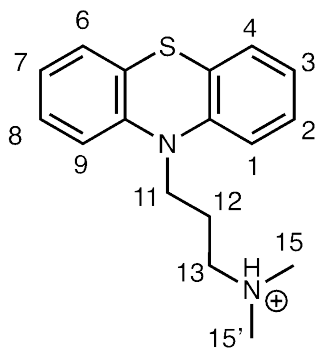
O-6Me-BCD-Phenothiazine.9.fid
O-6Me-BCD: TFP 6mM:4mM



O-6M-BCD.1.fid
Heptakis-(6-O-methyl)-BCD 10mM

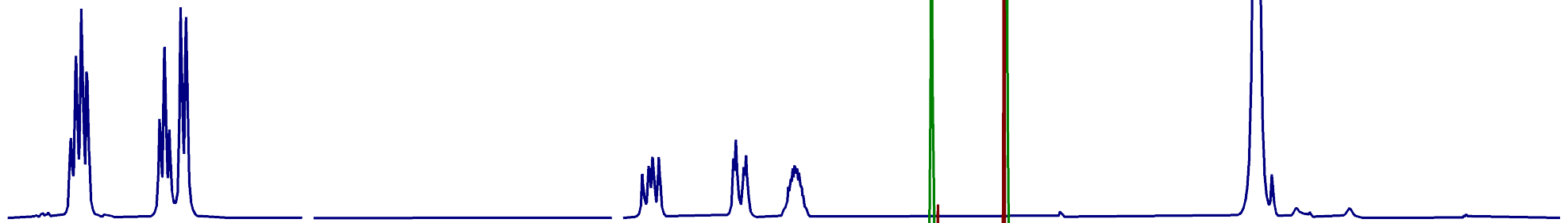


^1H NMR of DM- β -CD with Phenothiazines

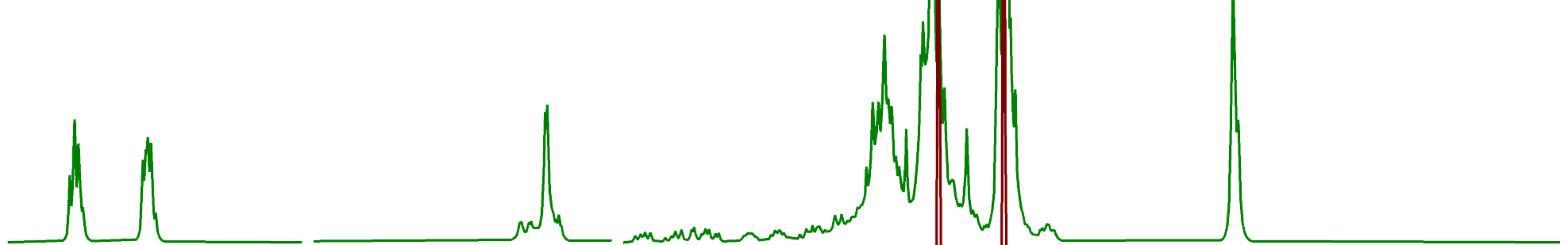


PMZ

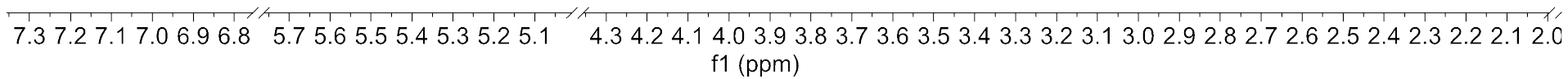
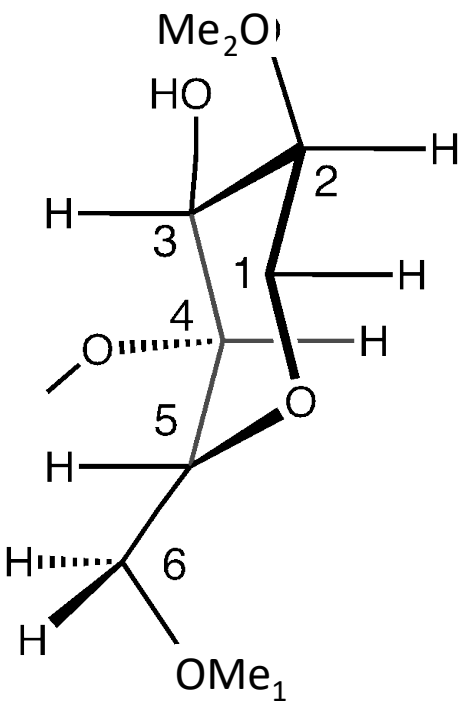
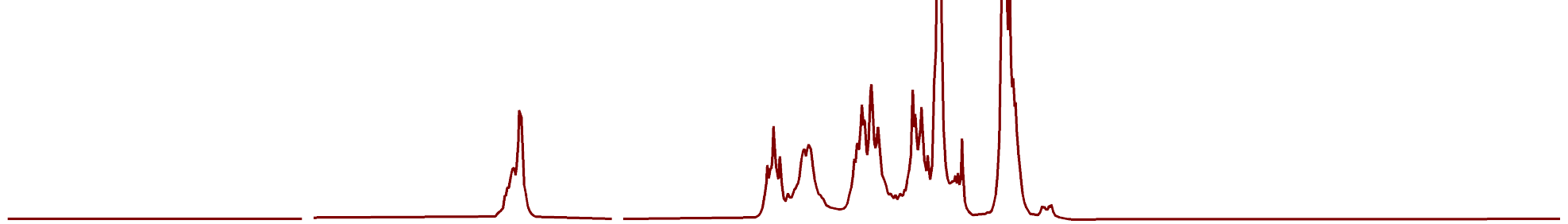
promethazine.1.fid
10mM Promethazine in D2O

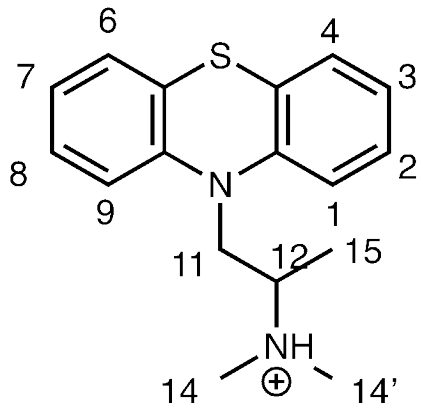


PMT-H26-BCD-NOSEY.1.fid

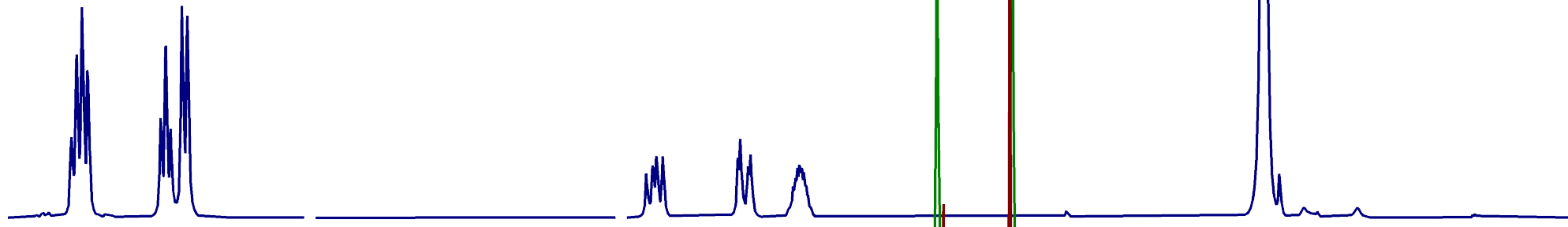


H26DM-BCD.1.fid
Heptakis-(2,6-dimethyl)-BCD 10mM



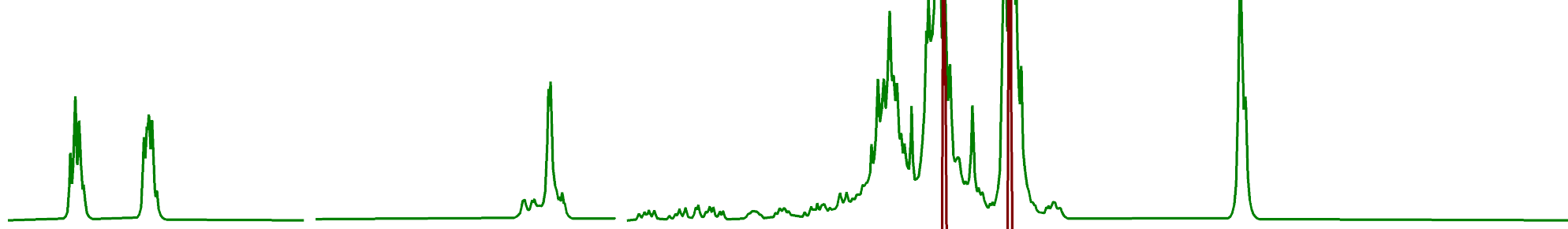


promethazine.1.fid
10mM Promethazine in D2O

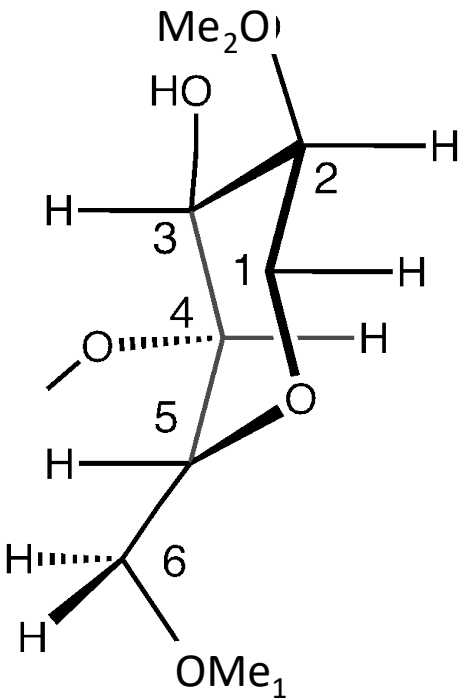
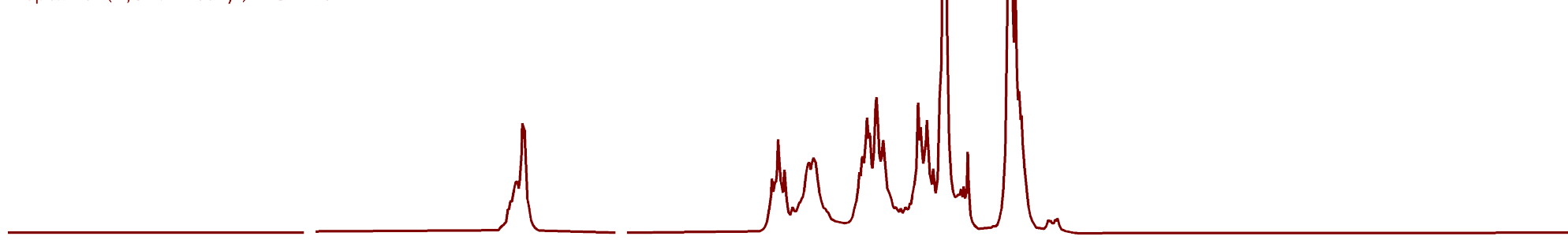


PMT-H26-BCD-NOSEY.1.fid

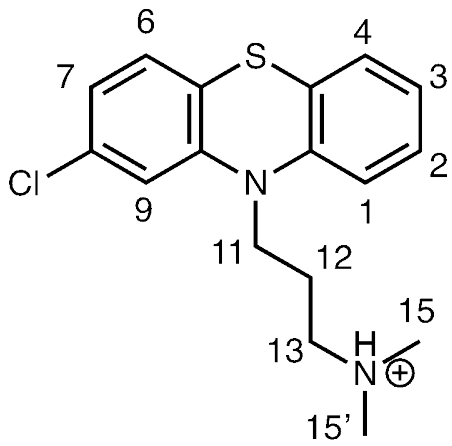
PMT



H26DM-BCD.1.fid
Heptakis-(2,6-dimethyl)-BCD 10mM

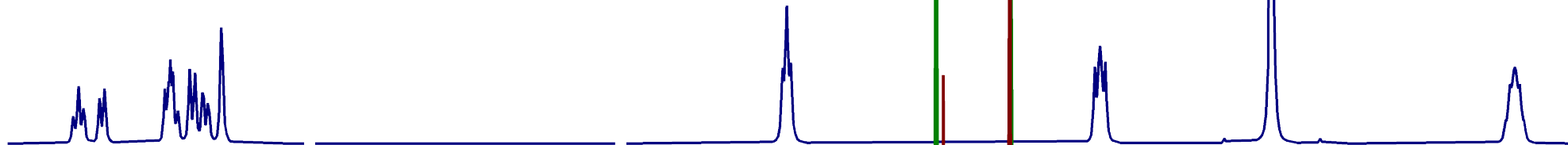


7.3 7.2 7.1 7.0 6.9 6.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0
f1 (ppm)

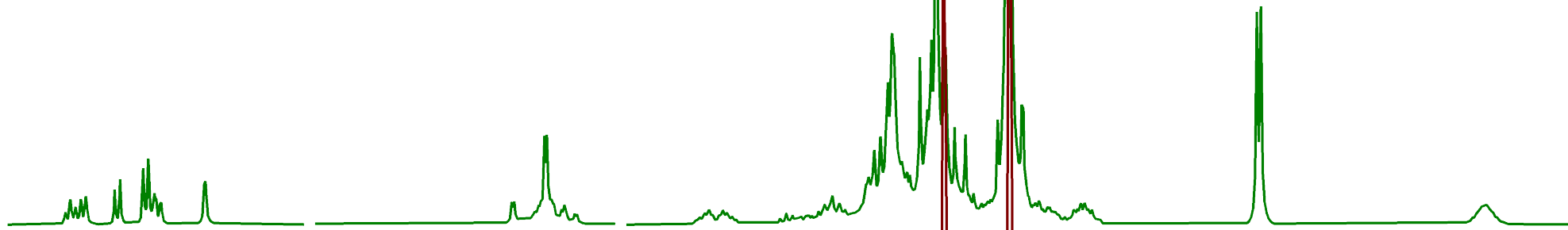


CPZ

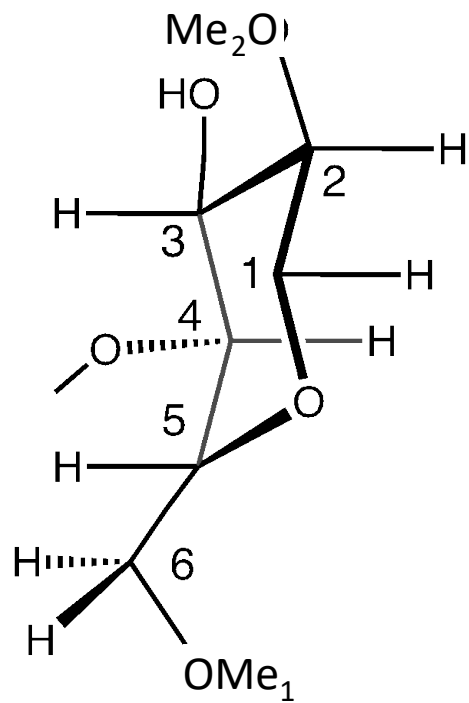
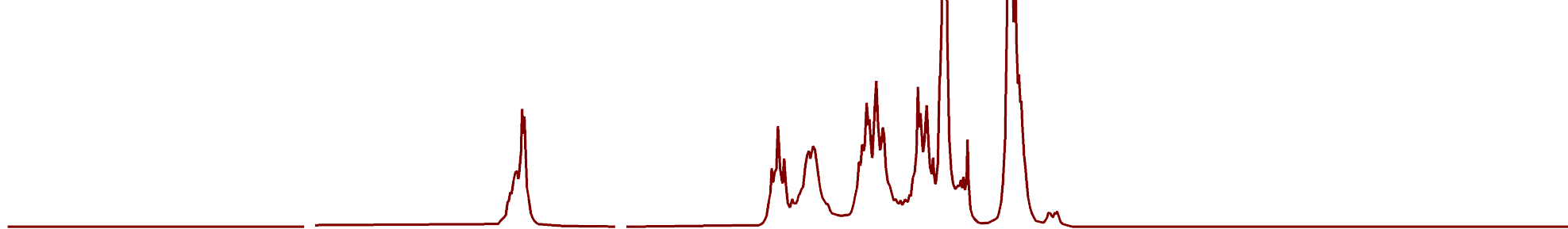
Chlorpromazine.1.fid
10mM Chlorpromazine in D2O



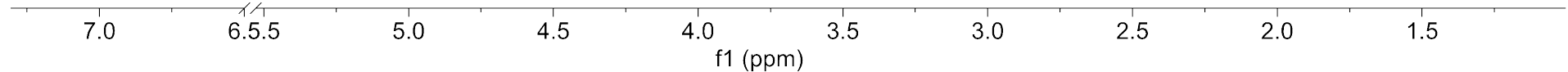
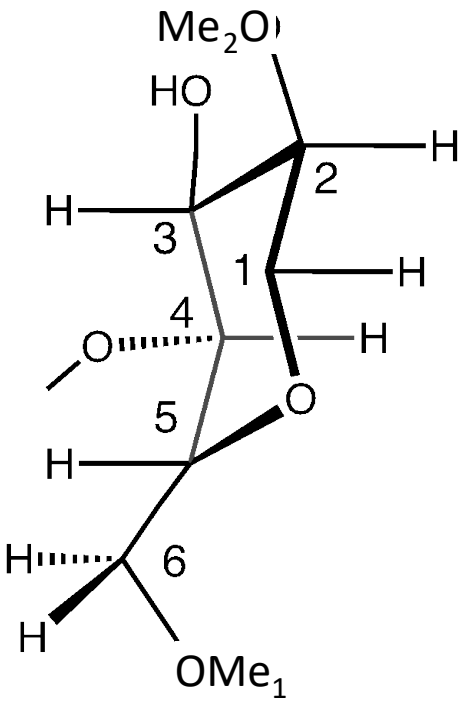
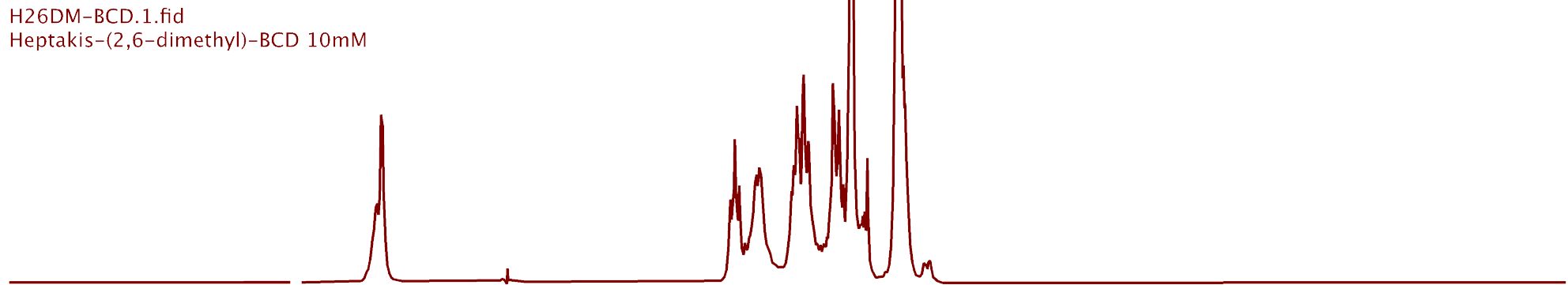
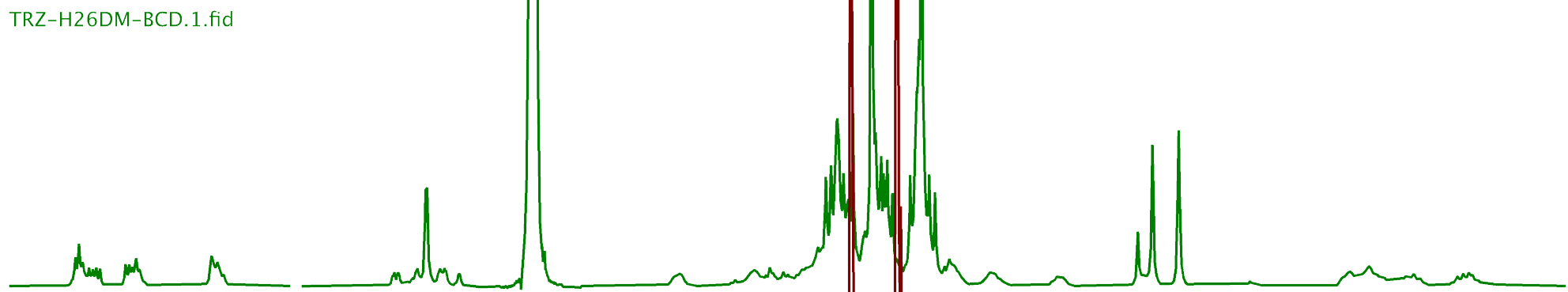
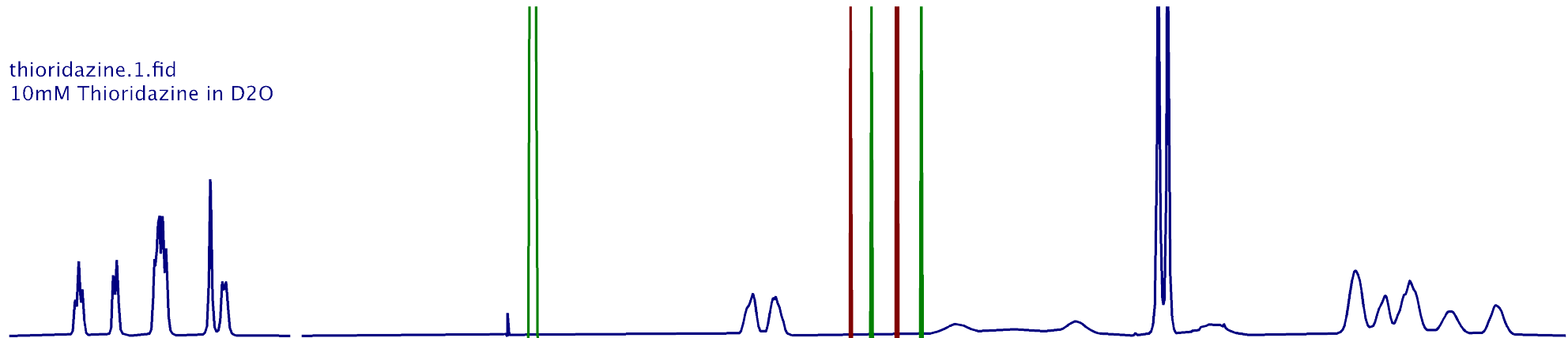
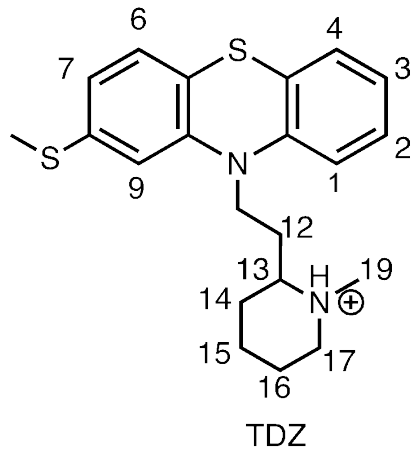
CPZ-H26DM-BCD.1.fid

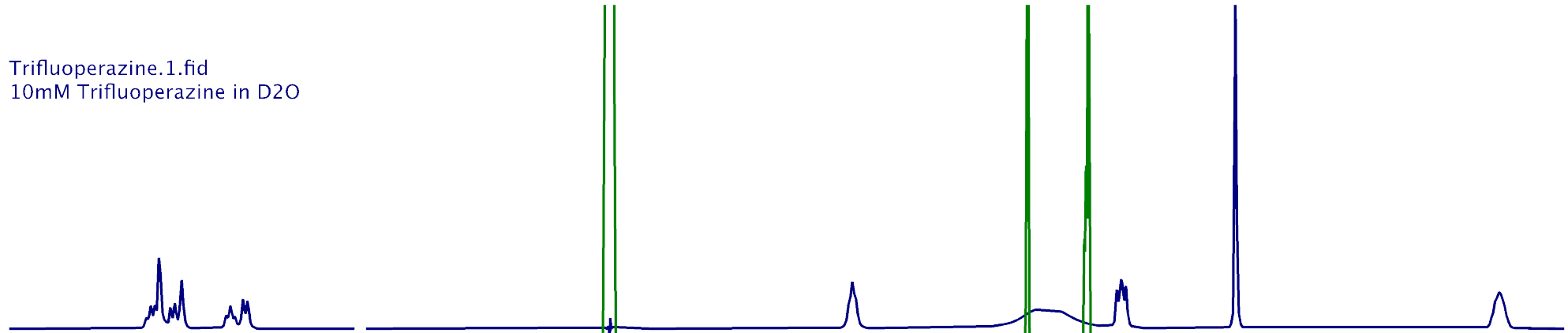
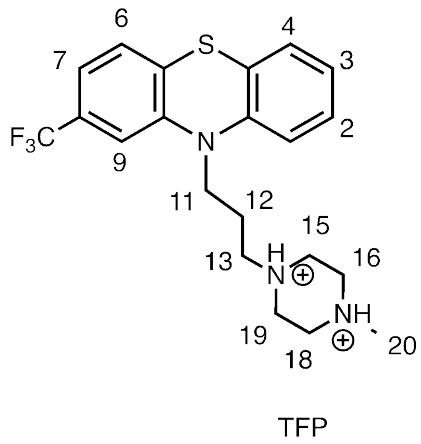


H26DM-BCD.1.fid
Heptakis-(2,6-dimethyl)-BCD 10mM

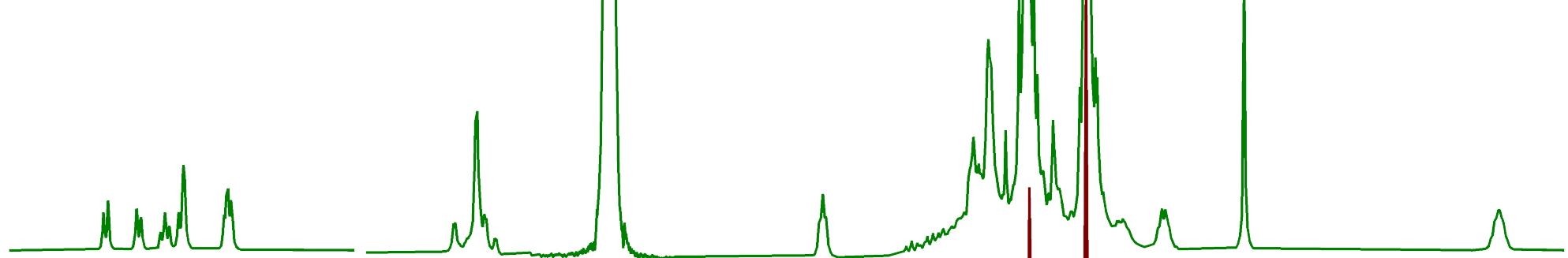


7.3 7.2 7.1 7.0 6.9 6.8 // 5.7 5.6 5.5 5.4 5.3 5.2 5.1 // 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.
f1 (ppm)





TFP-H26DM-BCD.1.fid



H26DM-BCD.1.fid
Heptakis-(2,6-dimethyl)-BCD 10mM

