

Multiple Intramolecular Hydrogen Bonding in Large Biomolecules: DFT Calculations and Deuterium Isotope Effects on ^{13}C Chemical Shifts as a Tool in Structural Studies

Poul Erik Hansen ^{1,*} and Fadhil S. Kamounah ²

¹ Department of Science and Environment, Roskilde University, DK-4000 Roskilde, Denmark

² Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark

* Correspondence: poulerik@ruc.dk

Table S1. Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

Number	Number	Type	X	Y	Z
1	6	0	-0.581627	1.390046	-0.194309
2	6	0	0.615643	2.075067	-0.416665
3	6	0	1.857150	1.374383	-0.364891
4	6	0	1.884942	-0.033754	-0.144182
5	6	0	0.653453	-0.728971	-0.008602
6	6	0	-0.572635	-0.024695	-0.029125
7	6	0	3.108671	2.138289	-0.570093
8	6	0	3.183300	-0.673119	-0.091082
9	6	0	4.351381	0.111603	-0.268463
10	6	0	4.371358	1.468680	-0.504953
11	6	0	5.638080	2.257205	-0.698411
12	1	0	6.519533	1.629359	-0.547234
13	1	0	5.692203	2.686778	-1.707210
14	1	0	5.687168	3.100859	0.000639
15	8	0	0.570440	3.394134	-0.699229
16	8	0	3.068283	3.394424	-0.798614
17	8	0	5.501108	-0.625315	-0.201299
18	8	0	0.581762	-2.074724	0.123564
19	7	0	-1.806353	2.097340	-0.202056
20	6	0	-1.781905	-0.829605	0.105835
21	6	0	3.606538	-2.000954	0.131859
22	8	0	2.966080	-3.061375	0.336946
23	1	0	1.486880	-2.505858	0.223536
24	1	0	-2.599345	1.540424	-0.514594
25	1	0	1.543354	3.661736	-0.796059
26	6	0	5.148529	-2.001812	0.097523
27	6	0	5.718415	-2.895455	-0.995855
28	1	0	5.460725	-3.936710	-0.782030
29	1	0	5.287753	-2.617846	-1.962191
30	1	0	6.805002	-2.797689	-1.065132
31	8	0	5.563778	-2.328170	1.395646

32 6 0 6.974888 -2.361590 1.626392
33 1 0 7.097624 -2.461777 2.706817
34 1 0 7.449081 -3.218494 1.133909
35 1 0 7.455406 -1.435350 1.293439
36 1 0 -1.630062 -1.876018 0.368459
37 7 0 -2.982958 -0.399520 -0.092684
38 6 0 -5.090791 -0.914389 0.830194
39 6 0 -4.415049 -1.884150 -1.253931
40 6 0 -6.130003 -2.004137 1.053388
41 1 0 -5.545379 -0.043068 0.327099
42 1 0 -4.737336 -0.581960 1.809743
43 6 0 -5.429910 -3.009874 -1.111322
44 1 0 -4.840554 -1.044757 -1.831663
45 1 0 -3.562752 -2.273890 -1.816500
46 1 0 -7.004979 -1.617013 1.577798
47 1 0 -5.711285 -2.844298 1.611020
48 1 0 -5.821626 -3.318371 -2.081856
49 1 0 -4.994134 -3.870839 -0.600876
50 1 0 -7.072243 -1.801746 -0.775553
51 7 0 -3.957815 -1.458095 0.075479
52 7 0 -6.606835 -2.564421 -0.269926
53 6 0 -7.617415 -3.658858 -0.089108
54 1 0 -8.456223 -3.264538 0.483997
55 1 0 -7.951980 -3.988327 -1.072728
56 1 0 -7.143643 -4.481333 0.446469
57 6 0 -2.091830 3.150493 0.642577
58 8 0 -1.288717 3.597475 1.460075
59 6 0 -3.476622 3.731844 0.473729
60 6 0 -3.862011 4.664517 1.353981
61 1 0 -4.837949 5.137500 1.291707
62 1 0 -3.199565 4.974188 2.155592
63 6 0 -4.363216 3.274393 -0.660076
64 1 0 -3.869575 3.397420 -1.631478
65 1 0 -4.632066 2.213666 -0.569229
66 1 0 -5.294170 3.848276 -0.674761

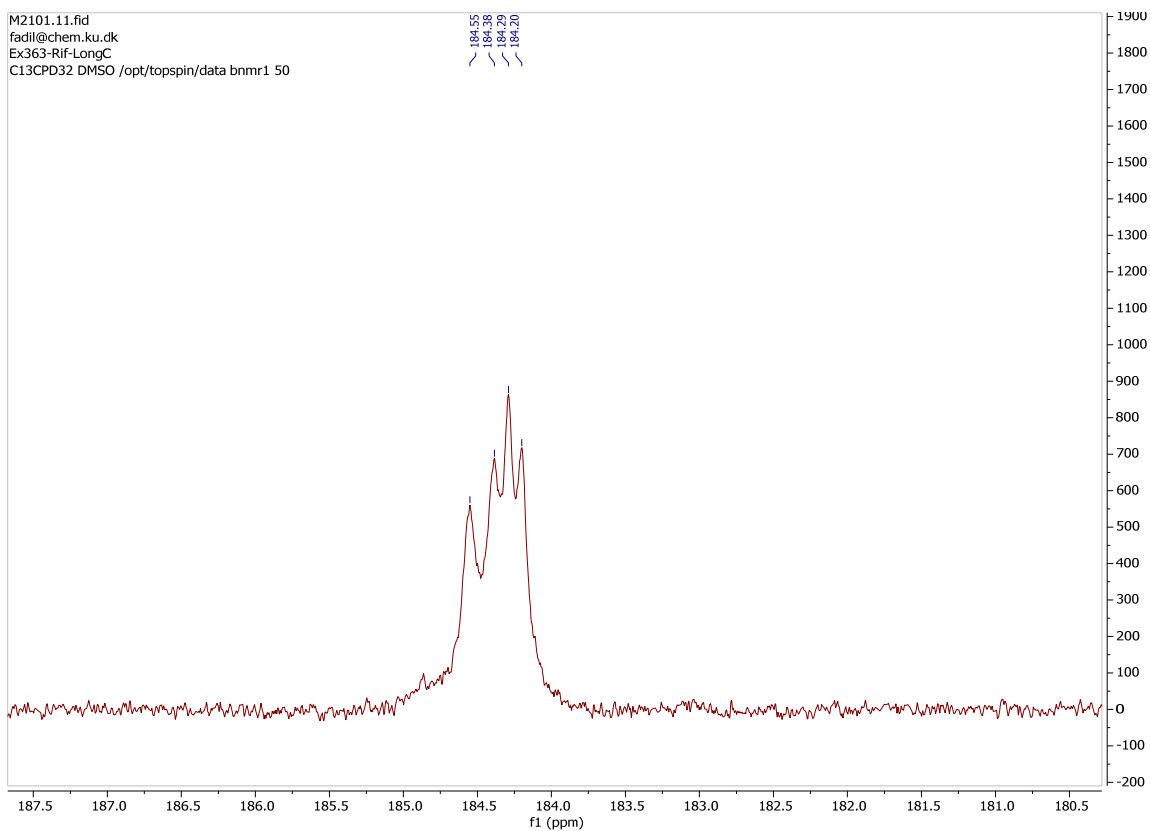
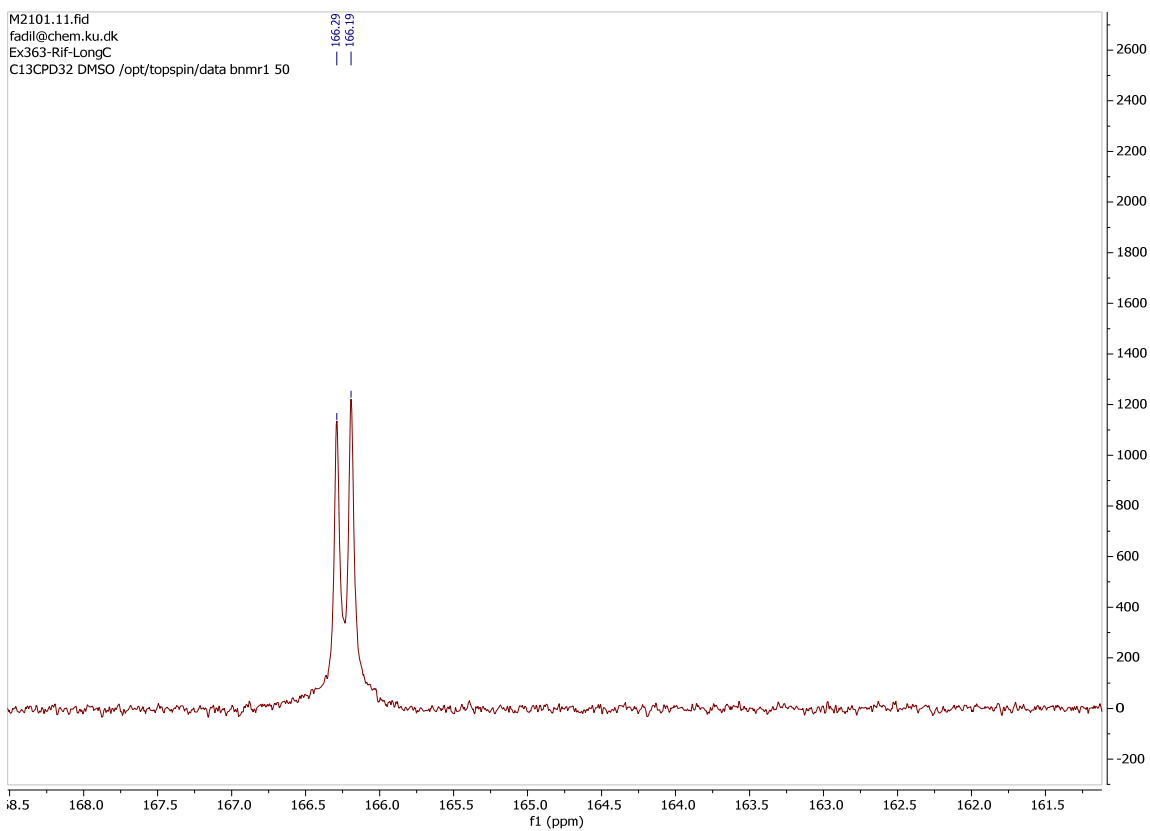
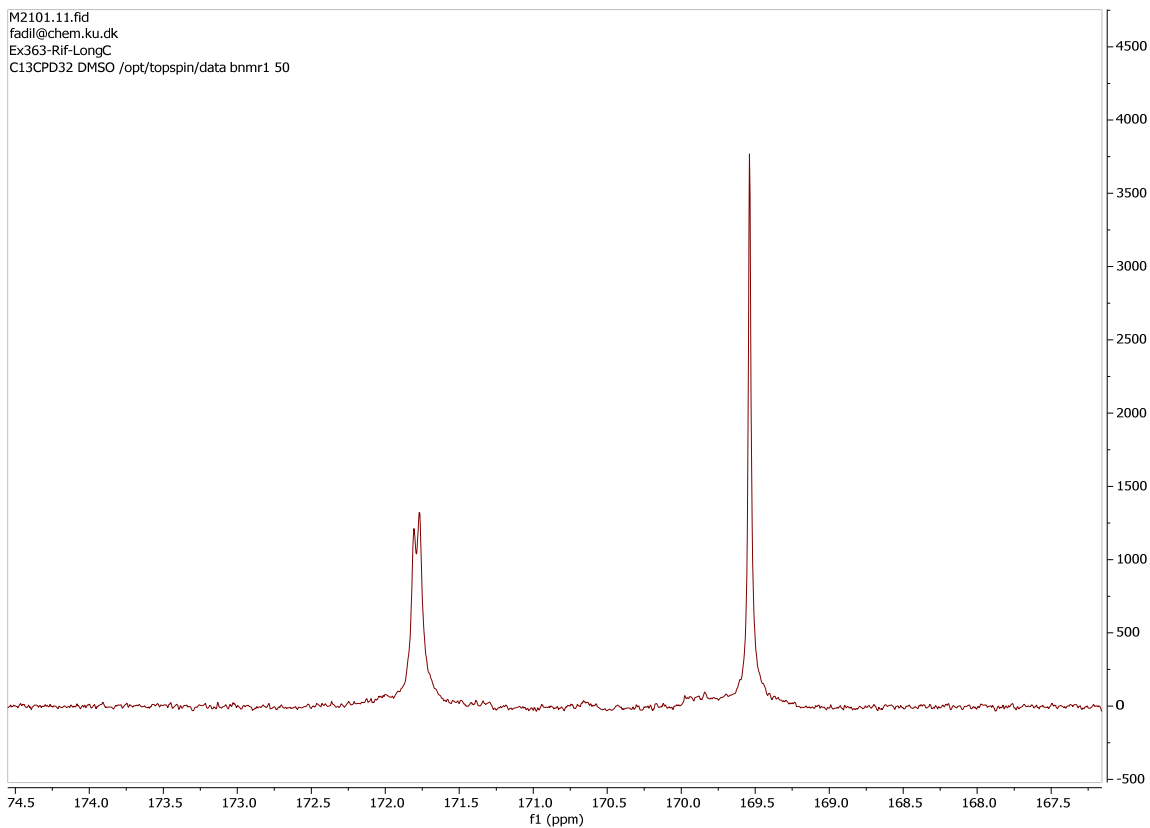
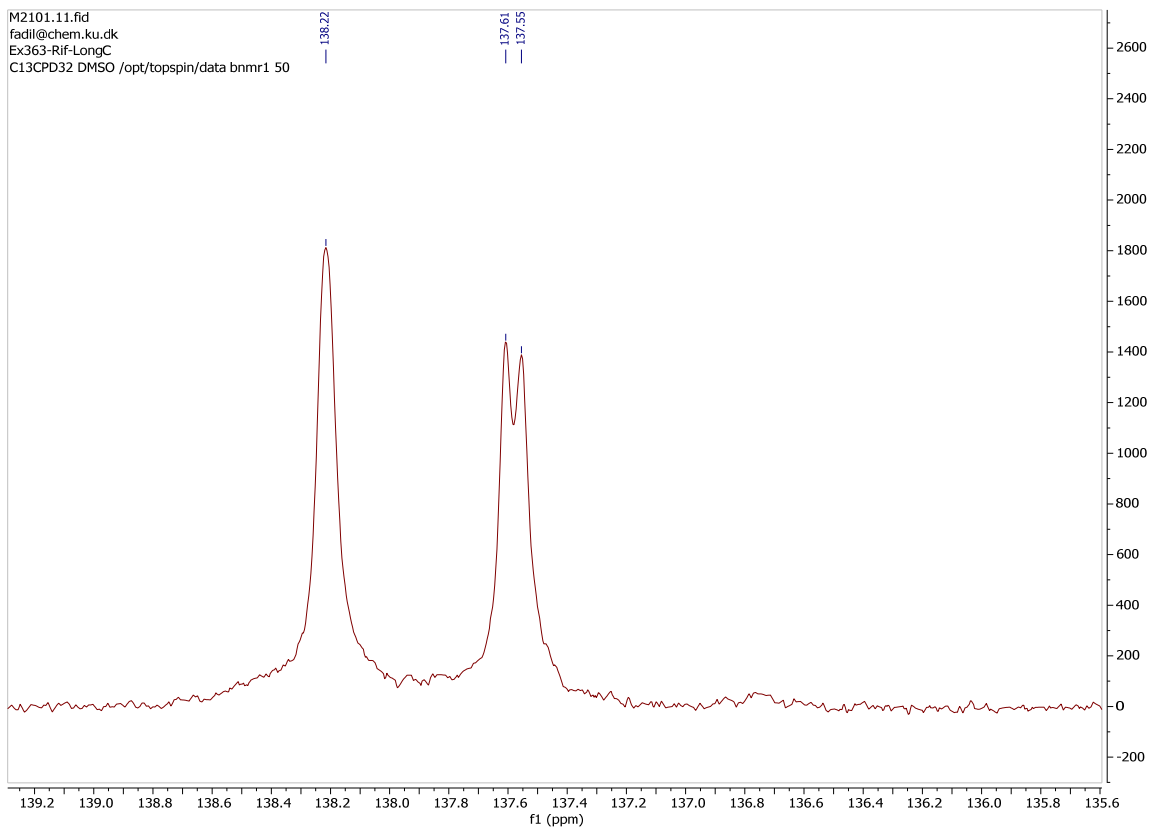
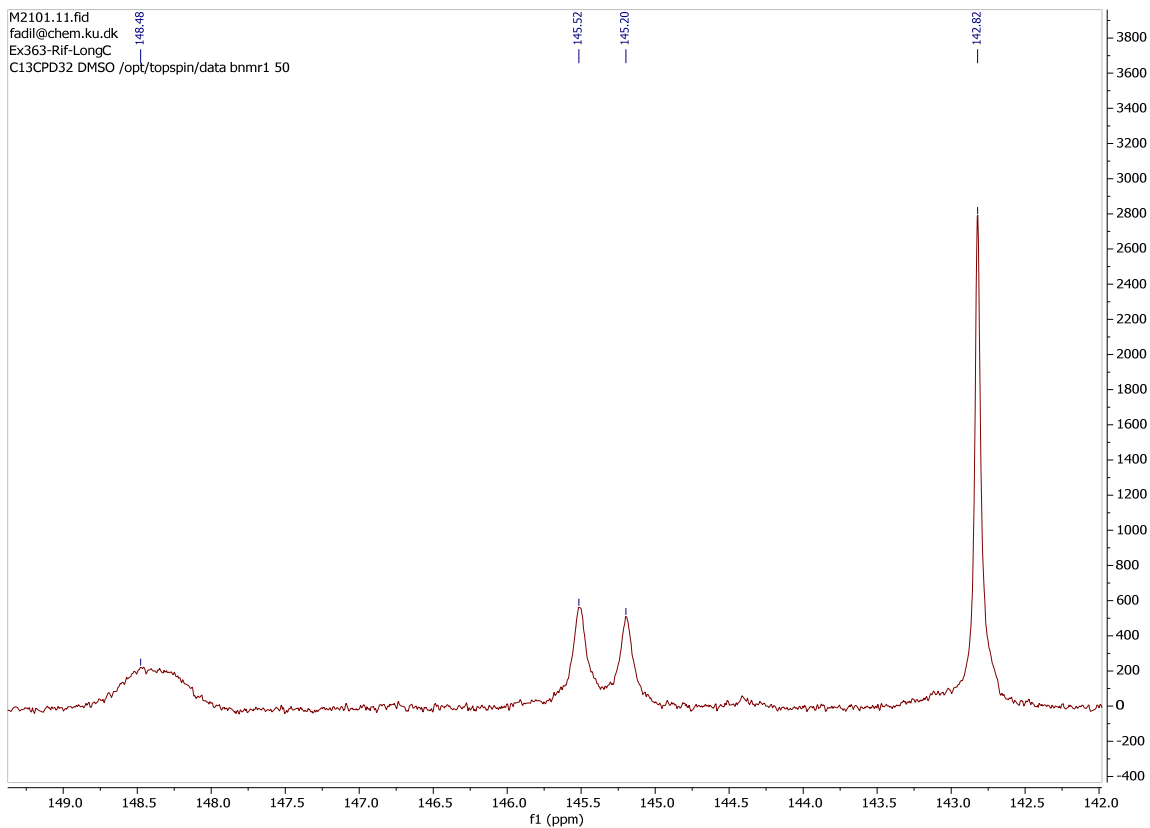
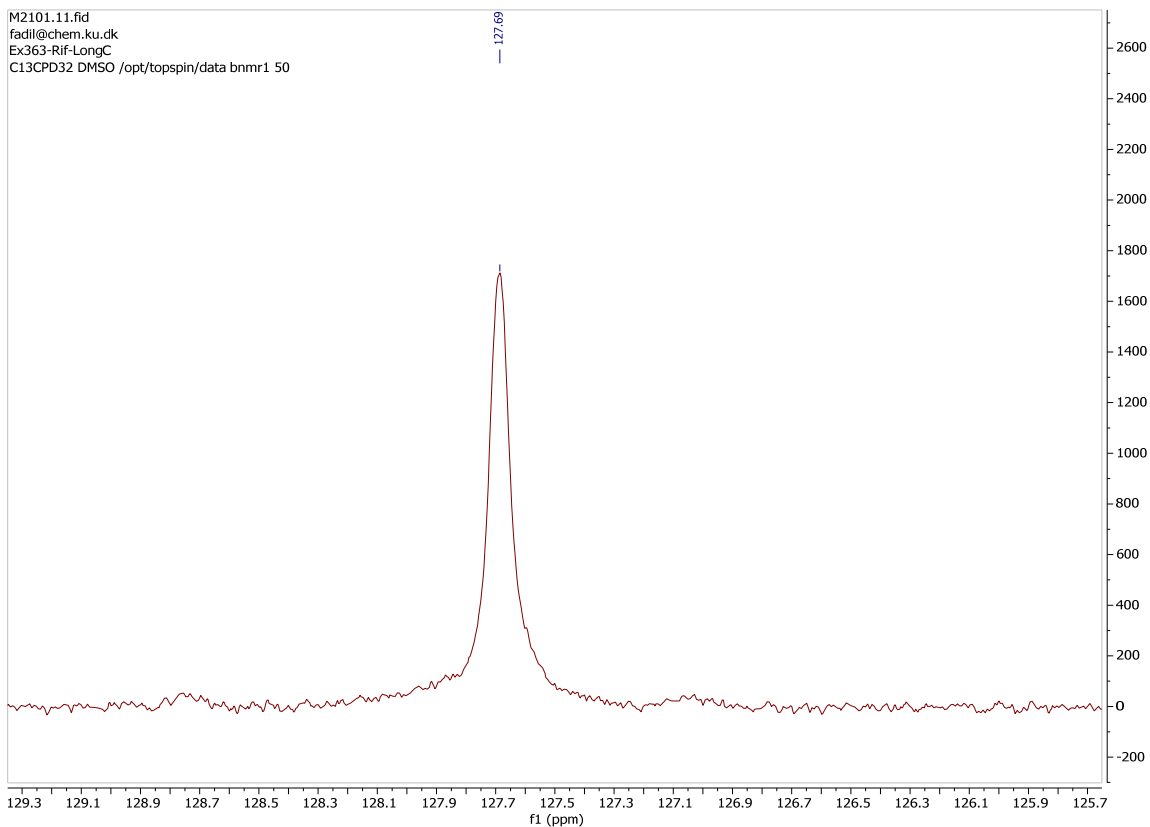
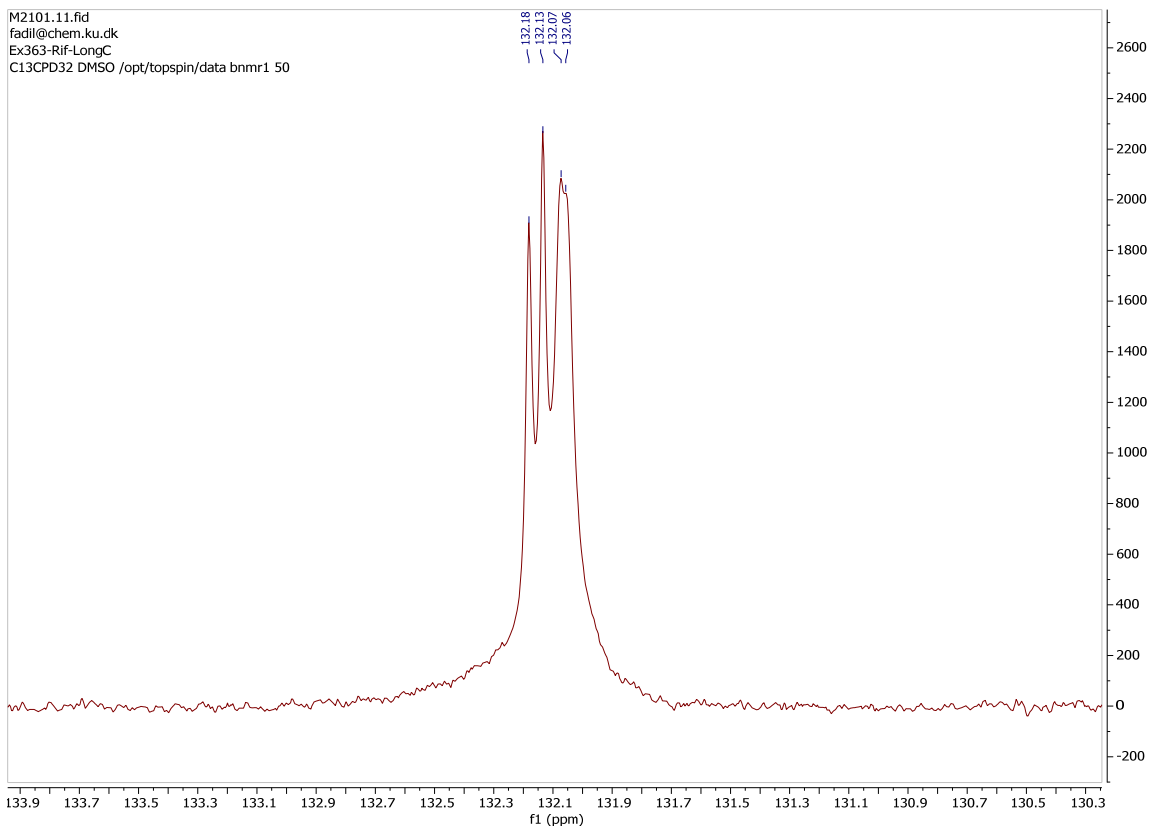
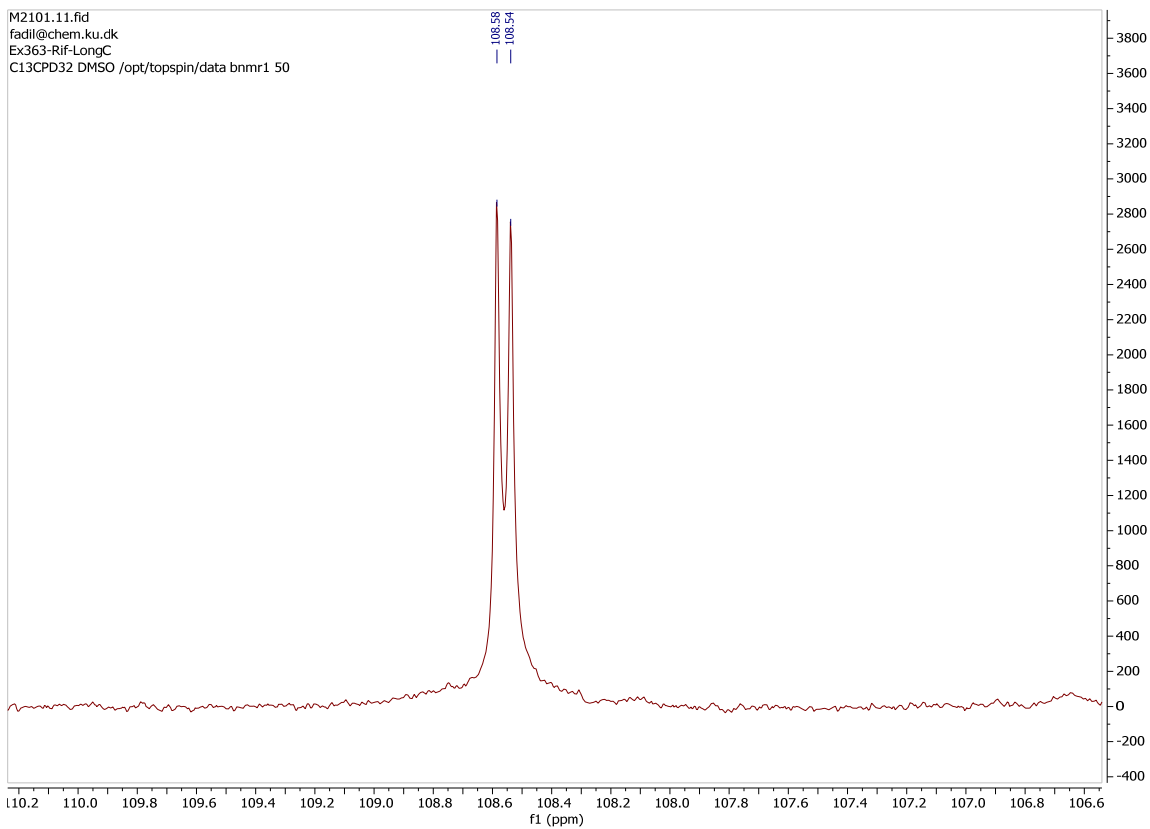
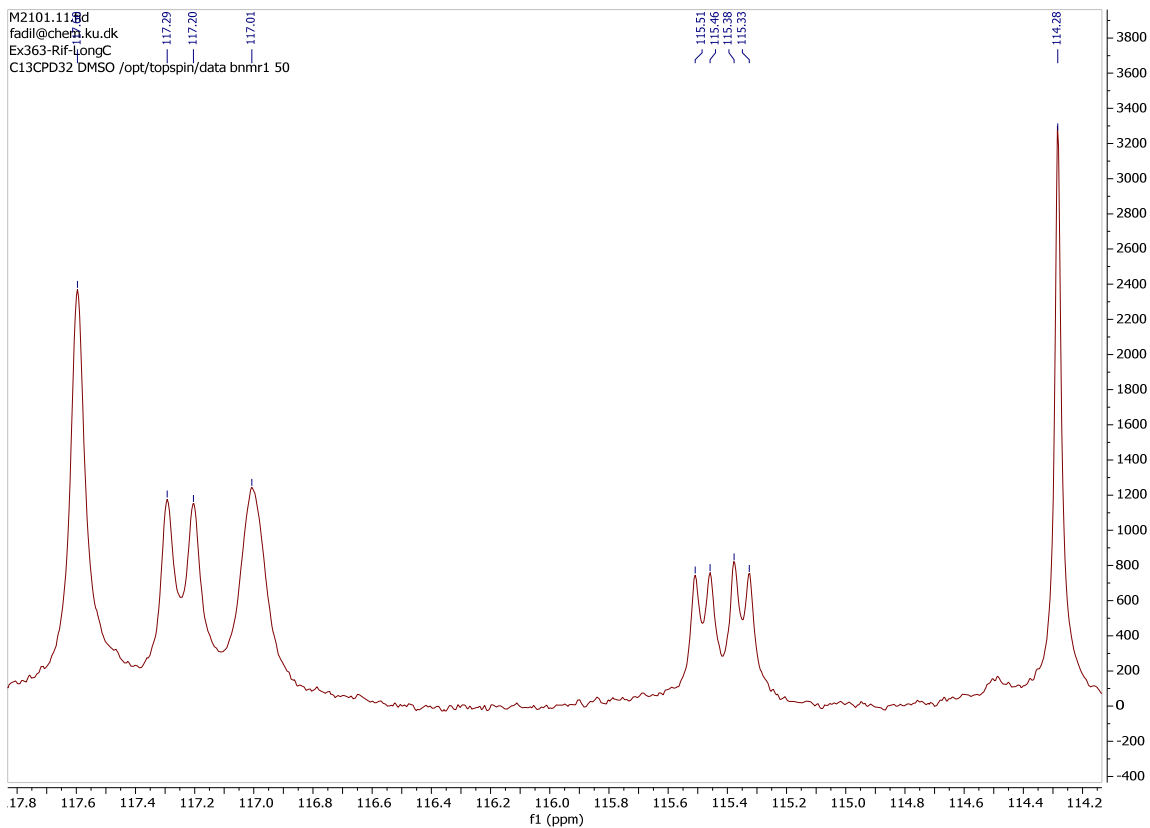


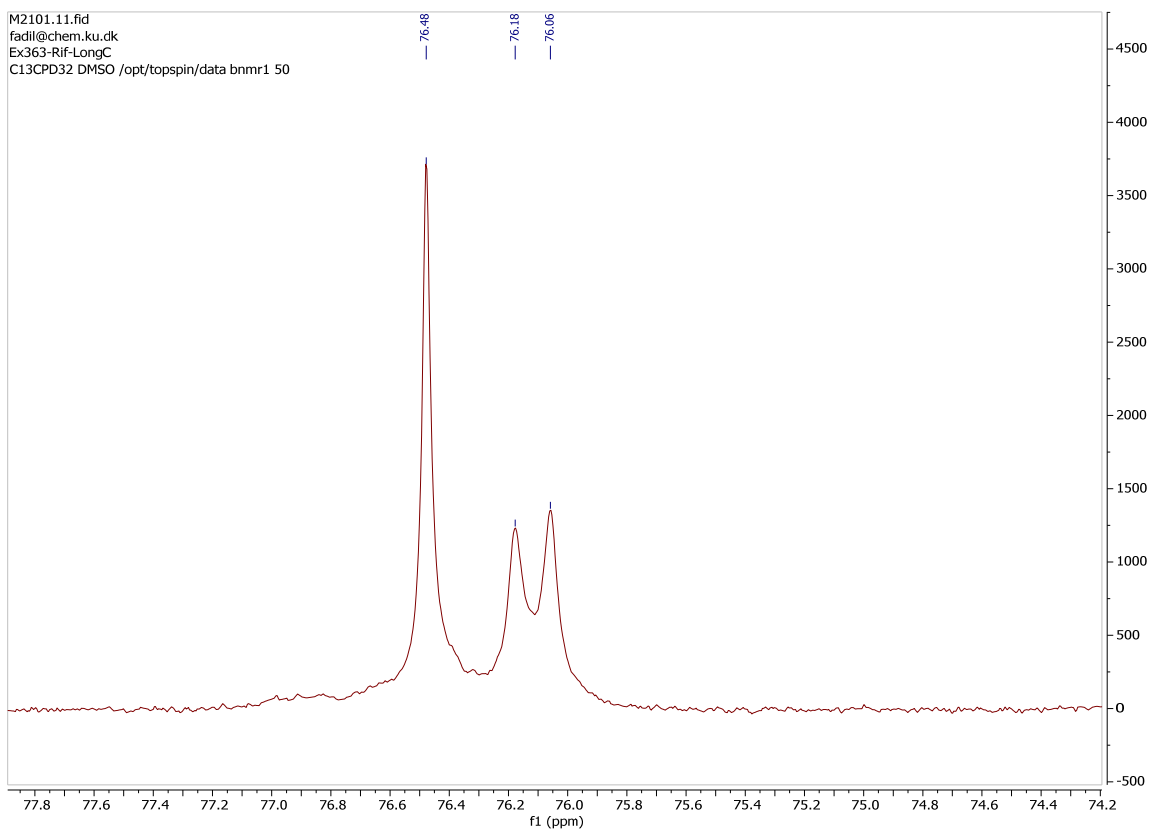
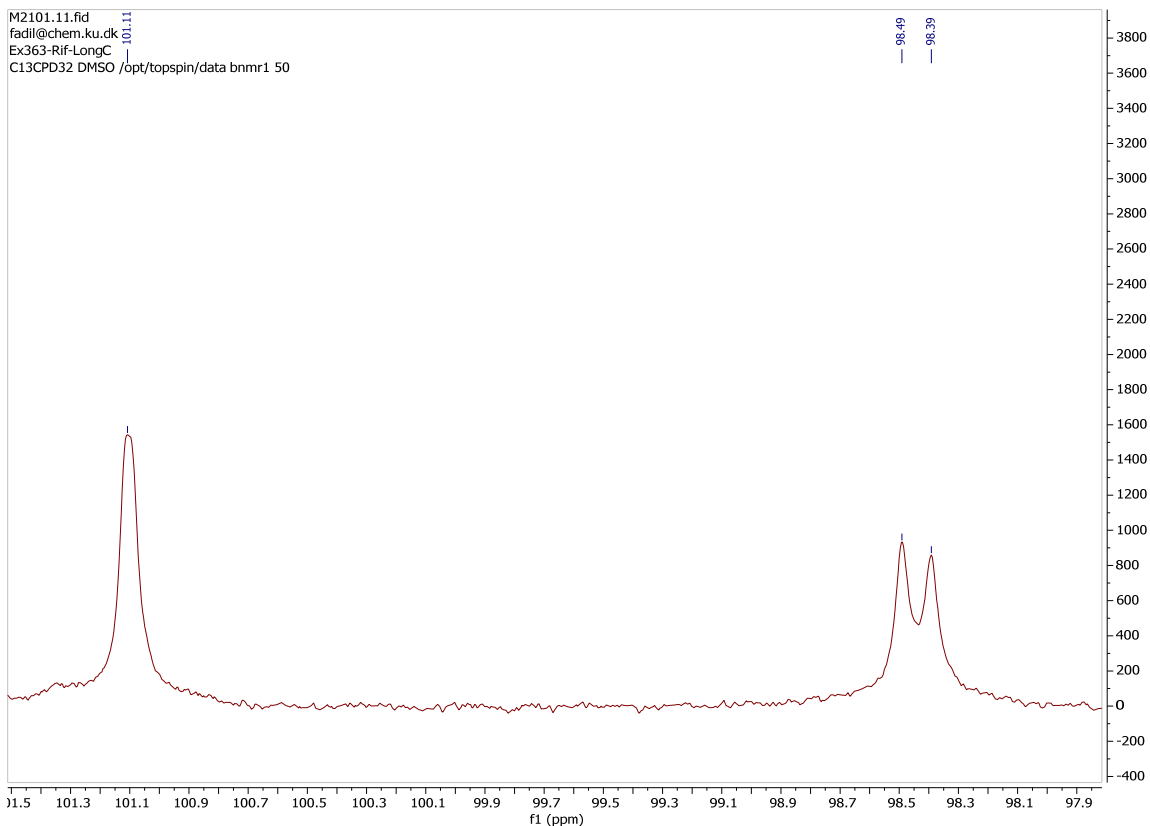
Figure S1. Expanded spectra of ^{13}C NMR spectrum of rifampicin.

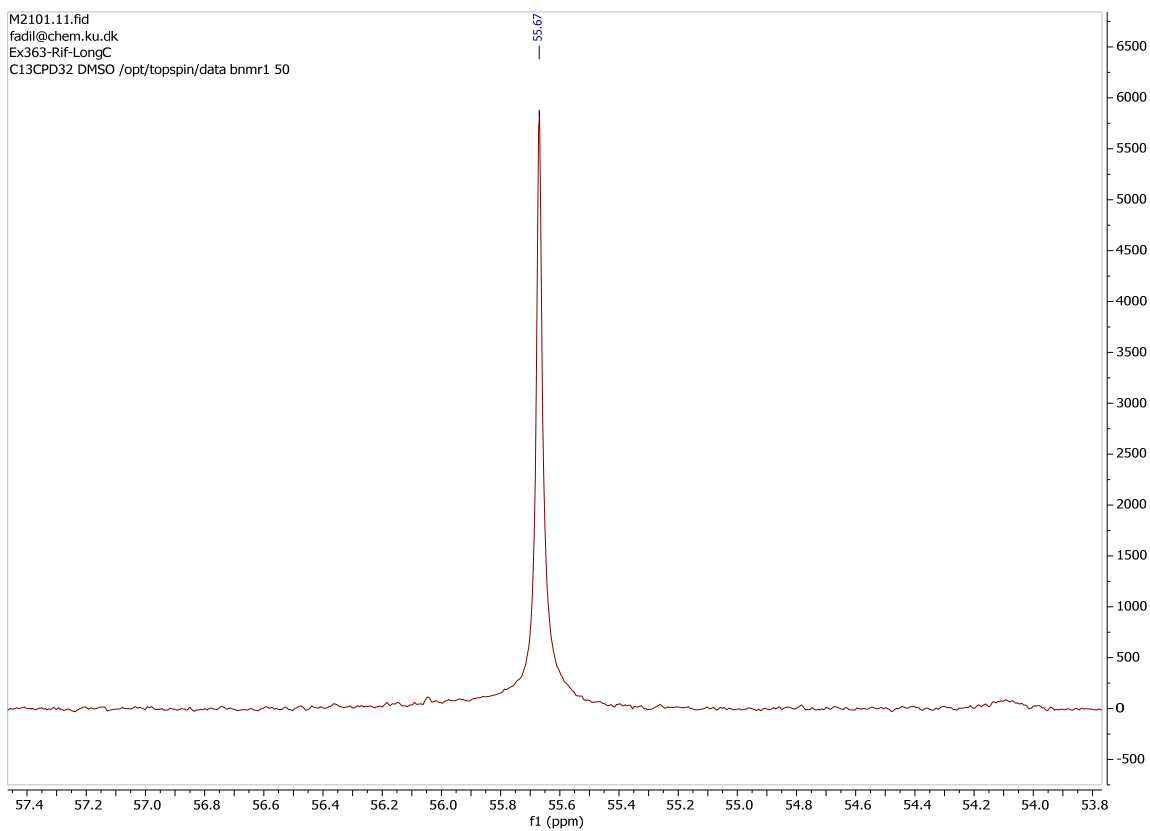
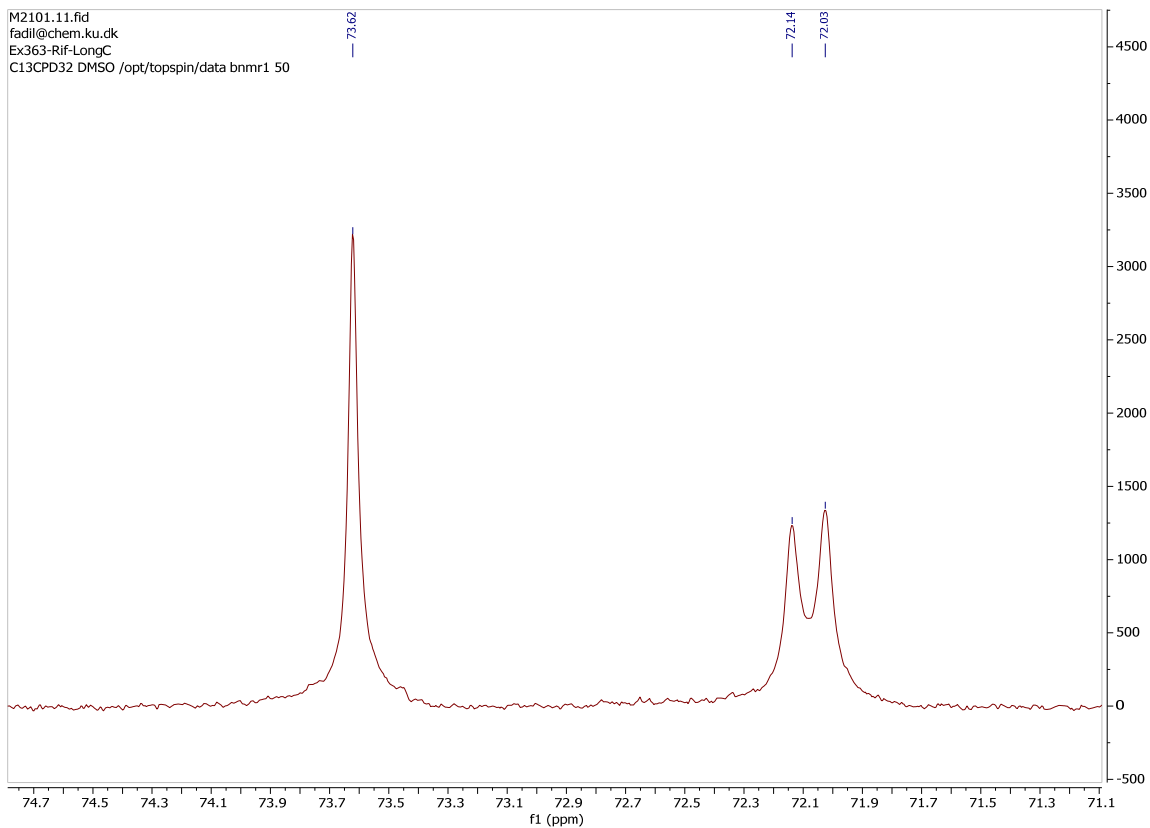


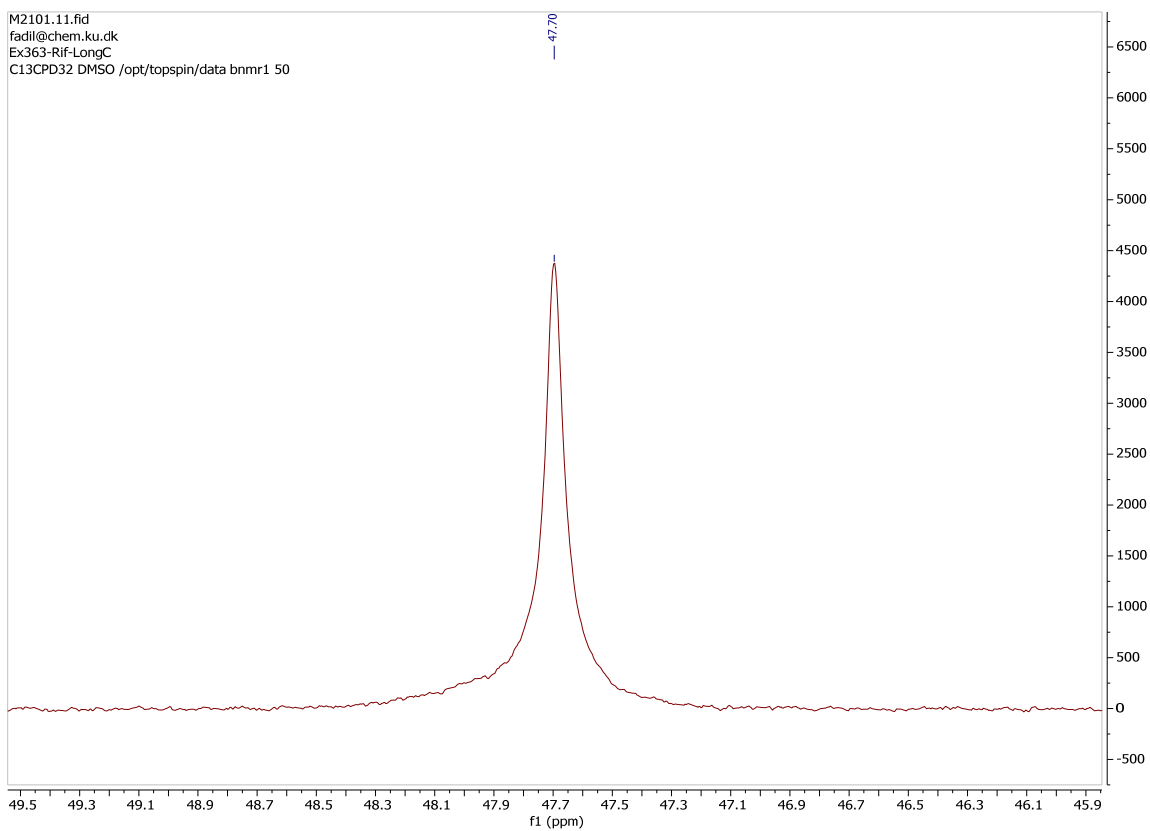
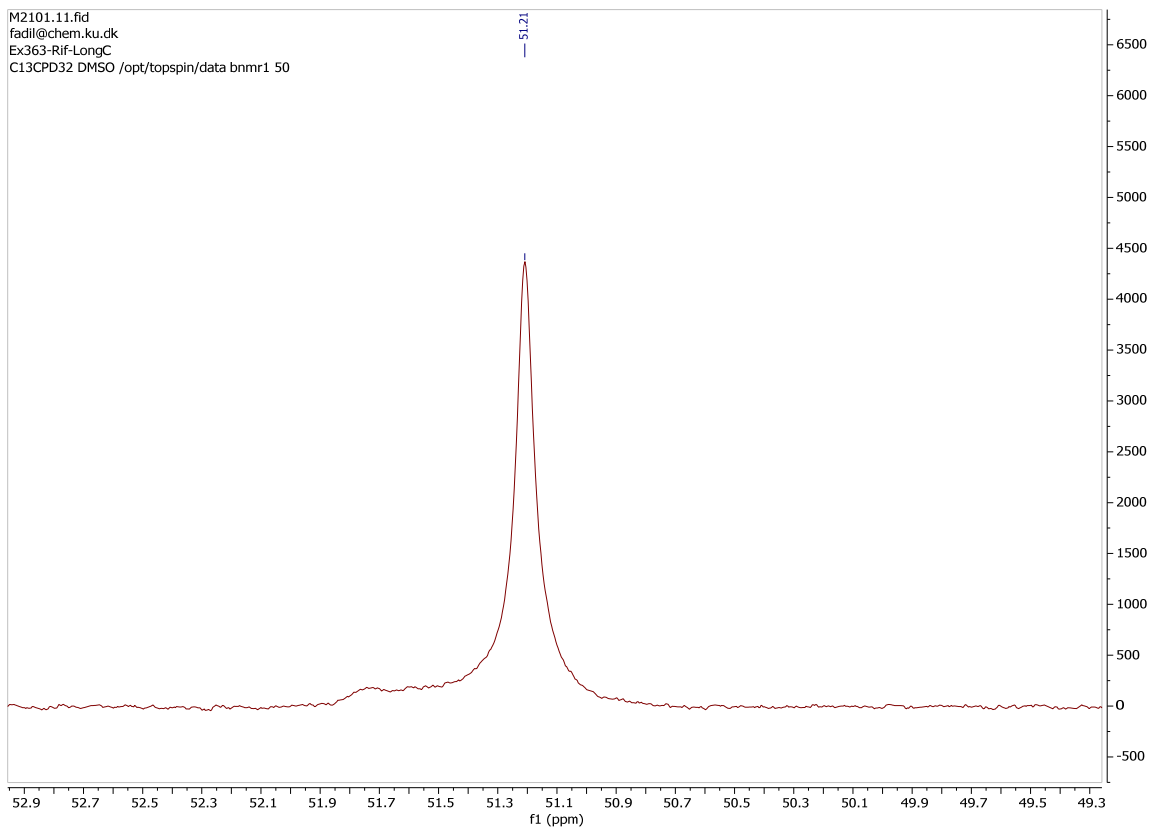


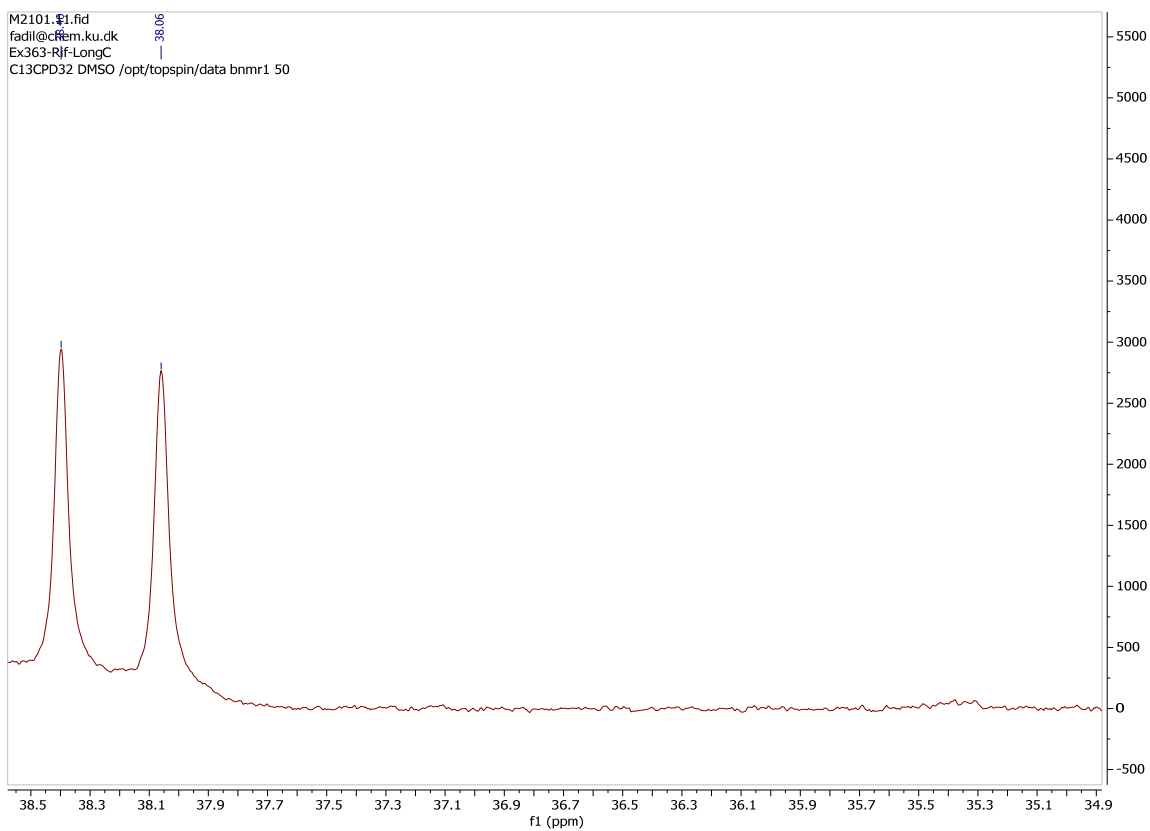
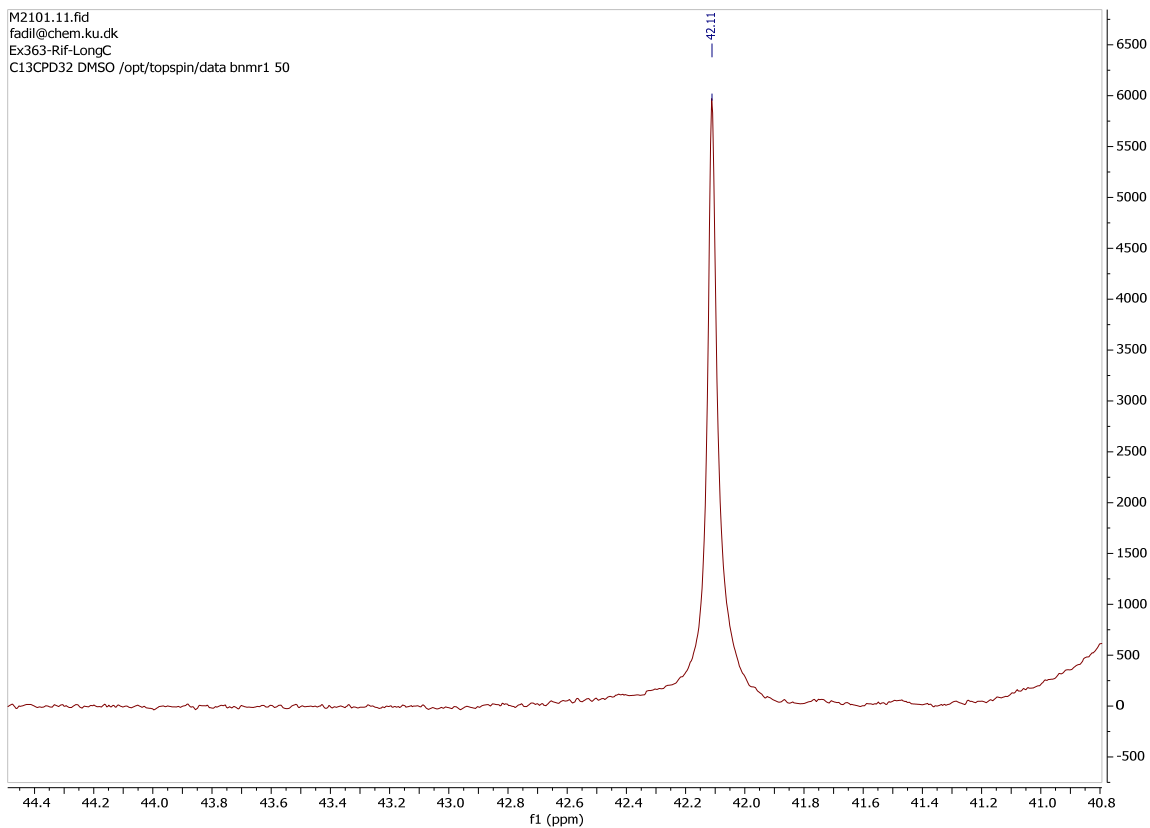


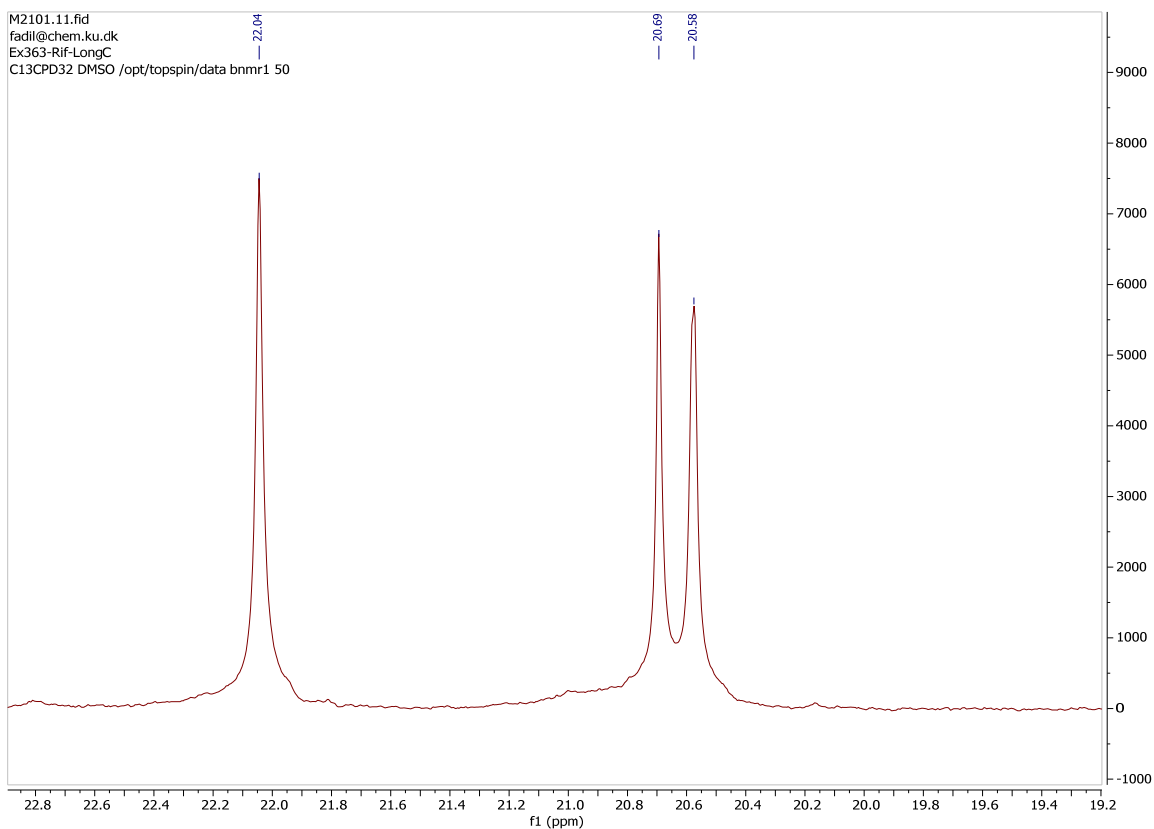
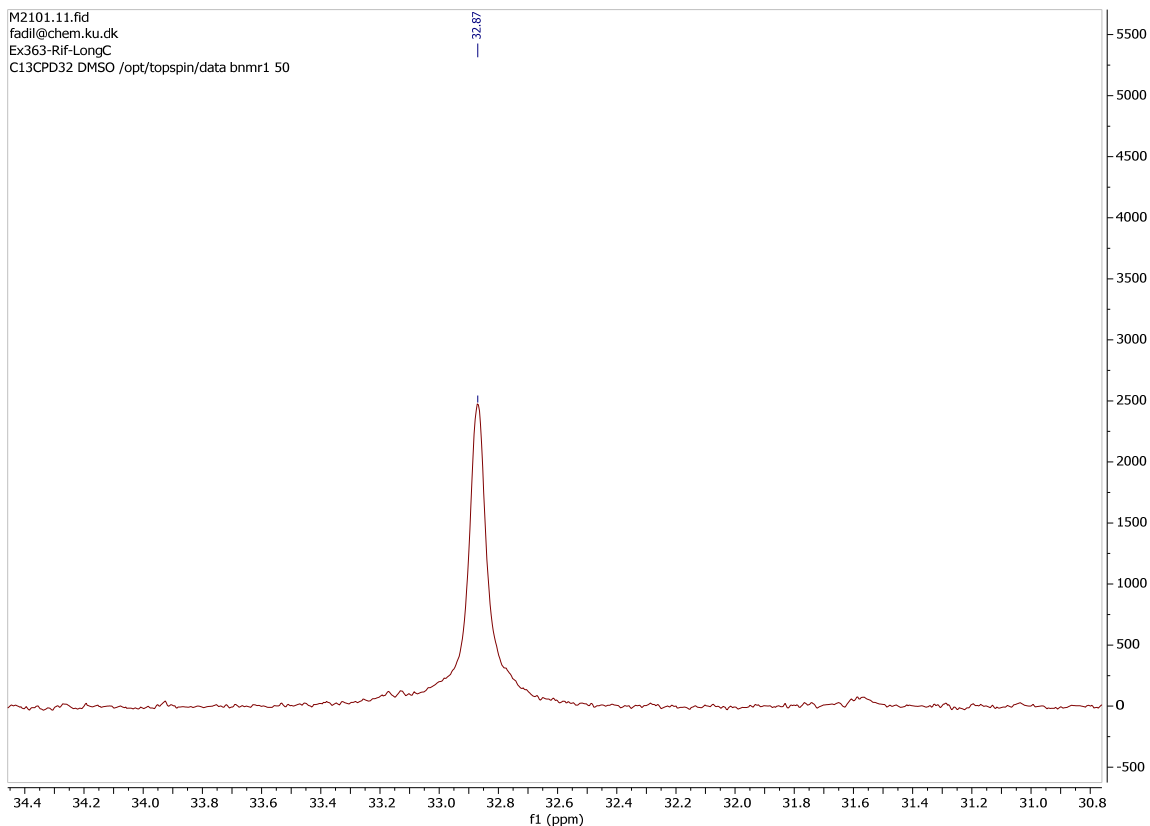


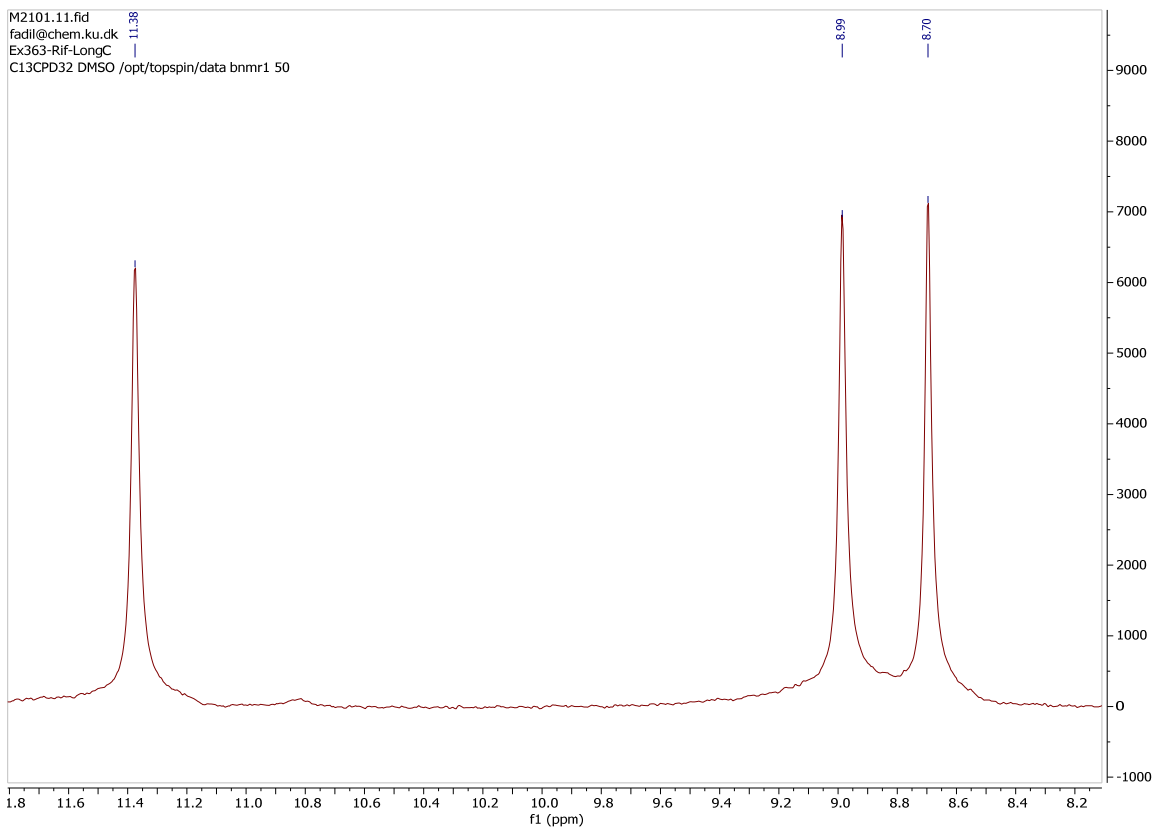
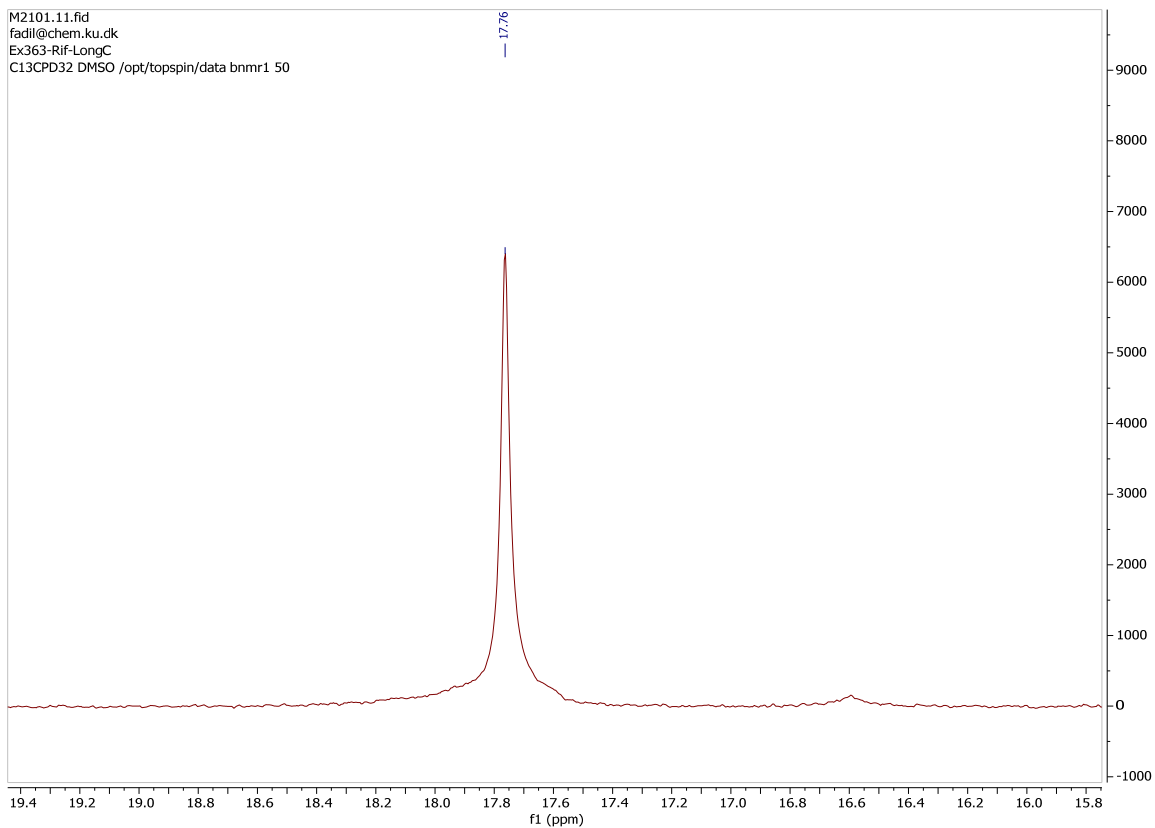












M2101.11.fid
fadli@chem.ku.dk
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