

Supporting Information

Boronic acids as phase-transfer reagents for Fischer glycosidations in low-polarity solvents

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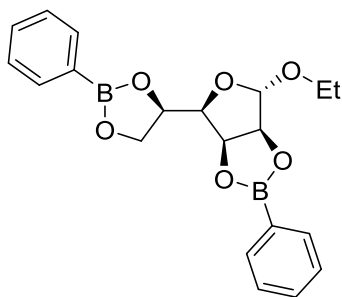
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Details of computational studies

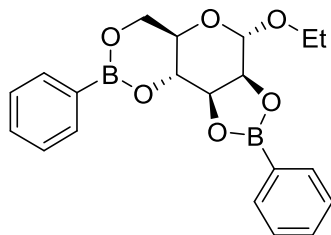
Electronic energies (hartree) and the number of imaginary frequencies are given, and the frequency (cm^{-1}) where applicable, for each structure. Total electronic energies for the structures were calculated using B3LYP/6-31+G(d,p) in the gas phase (indicated below). Energies for all possible boronic esters between phenylboronic acid and the *cis*-1,2- or 1,3-diol(s) of each monosaccharide was calculated for furanoside and pyranoside isomers. Only the lowest energy structures for each isomer are shown below.



Ethyl α -D-mannofuranoside (bis-boronate)

Energy: -1276.71041055
Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.018344	1.227902	0.040521
2	6	0	-1.918019	2.481427	-0.004777
3	6	0	-2.149366	1.461194	1.124300
4	6	0	-0.872897	0.565676	1.105900
5	1	0	0.675606	1.956910	0.536546
6	1	0	-2.796487	2.622702	-0.645175
7	1	0	-2.351213	1.963337	2.071825
8	1	0	-0.362626	0.469684	2.066243
9	8	0	-0.902199	1.915067	-0.826351
10	8	0	-1.518578	3.686361	0.593767
11	6	0	-1.345121	4.778809	-0.321192
12	1	0	-0.556212	4.532972	-1.042526
13	1	0	-2.281392	4.927121	-0.880825
14	6	0	-0.989093	6.018616	0.479739
15	1	0	-0.856337	6.873189	-0.192027
16	1	0	-1.780457	6.259792	1.195868
17	1	0	-0.057229	5.867927	1.033384
18	8	0	-3.230840	0.578281	0.808160
19	8	0	-1.348591	-0.728102	0.706863
20	6	0	0.867621	0.293647	-0.807492
21	1	0	0.235077	-0.500113	-1.215029
22	6	0	1.675722	1.013336	-1.917984
23	1	0	1.299468	0.798306	-2.920407
24	1	0	1.701347	2.099211	-1.775700
25	8	0	3.013920	0.496126	-1.791265
26	5	0	-2.715680	-0.675192	0.549154
27	8	0	1.872867	-0.313210	0.028178
28	5	0	3.087935	-0.220693	-0.619486
29	6	0	-3.583281	-1.893701	0.138767
30	6	0	-4.979259	-1.773694	0.001333
31	6	0	-2.995081	-3.150341	-0.100197
32	6	0	-5.762049	-2.870744	-0.362539
33	1	0	-5.450390	-0.811680	0.183234
34	6	0	-3.773744	-4.250068	-0.464887
35	1	0	-1.919355	-3.262069	0.004070
36	6	0	-5.159087	-4.110770	-0.596426
37	1	0	-6.838289	-2.761570	-0.463427
38	1	0	-3.304214	-5.213042	-0.645252
39	1	0	-5.766917	-4.965886	-0.879456
40	6	0	4.395992	-0.858819	-0.078315
41	6	0	4.390949	-1.624199	1.103197
42	6	0	5.617518	-0.689833	-0.757452
43	6	0	5.565071	-2.200403	1.591646
44	1	0	3.456178	-1.767755	1.638109
45	6	0	6.794241	-1.264246	-0.273241
46	1	0	5.639603	-0.103284	-1.671769
47	6	0	6.768885	-2.020509	0.902978
48	1	0	5.543376	-2.789119	2.504579
49	1	0	7.728676	-1.124357	-0.809692
50	1	0	7.683807	-2.468723	1.280993

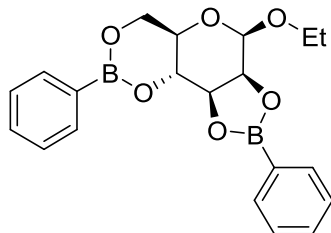


Ethyl α -D-mannopyranoside (bis-boronate)

Energy: -1276.70709953

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.196424	-2.687916	-0.146628
2	6	0	1.641616	-1.491832	0.711586
3	6	0	0.613707	-0.345837	0.911079
4	6	0	-0.383957	-0.226257	-0.241240
5	6	0	-0.842996	-1.607206	-0.705687
6	1	0	1.957339	-1.891747	1.680916
7	1	0	2.064834	-3.099660	-0.675593
8	1	0	0.065521	-0.442964	1.851760
9	1	0	0.115630	0.271585	-1.083043
10	1	0	-1.318961	-2.141923	0.128638
11	8	0	0.286285	-2.338379	-1.180625
12	8	0	0.649978	-3.629674	0.742949
13	6	0	0.403063	-4.923395	0.170602
14	1	0	1.337322	-5.300548	-0.272234
15	1	0	-0.338432	-4.837629	-0.633099
16	6	0	-0.087545	-5.844699	1.273153
17	1	0	-1.014863	-5.464700	1.712805
18	1	0	-0.283084	-6.842626	0.866945
19	1	0	0.659268	-5.933945	2.067841
20	8	0	2.771630	-0.830940	0.111857
21	8	0	1.443554	0.830301	0.972838
22	5	0	2.658495	0.516569	0.398128
23	6	0	3.767684	1.558024	0.099650
24	6	0	3.553726	2.927962	0.345272
25	6	0	5.012763	1.160232	-0.423765
26	6	0	4.548953	3.869249	0.076783
27	1	0	2.598470	3.251952	0.748939
28	6	0	6.010711	2.098092	-0.694105
29	1	0	5.195179	0.107077	-0.619012
30	6	0	5.779044	3.454474	-0.443625
31	1	0	4.368038	4.922678	0.271360
32	1	0	6.966111	1.775062	-1.098148
33	1	0	6.554788	4.185931	-0.653397
34	6	0	-1.841958	-1.451017	-1.844928
35	1	0	-2.297150	-2.410723	-2.104668
36	1	0	-1.334782	-1.056705	-2.733802
37	8	0	-2.892817	-0.559411	-1.461273
38	8	0	-1.506860	0.559364	0.159261
39	5	0	-2.713015	0.394550	-0.486997
40	6	0	-3.915985	1.308311	-0.089981
41	6	0	-3.767257	2.322906	0.874739
42	6	0	-5.179816	1.142712	-0.687659
43	6	0	-4.840724	3.141704	1.231066
44	1	0	-2.798778	2.468183	1.344893
45	6	0	-6.257057	1.957849	-0.334874
46	1	0	-5.313076	0.365953	-1.435298
47	6	0	-6.088413	2.959677	0.626282
48	1	0	-4.706435	3.920387	1.976954
49	1	0	-7.225302	1.814451	-0.806809
50	1	0	-6.925089	3.596021	0.902037

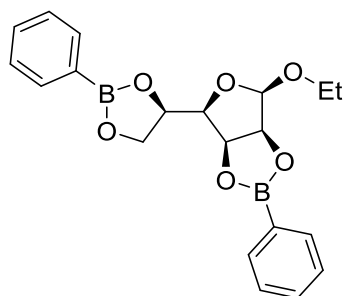


Ethyl β -D-mannopyranoside (bis-boronate)

Energy: -1276.70021333

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	1.414494	-2.431769	0.642730
2	6	O	1.648620	-1.022834	1.202064
3	6	O	0.391867	-0.109175	1.218623
4	6	O	-0.563100	-0.385897	0.053007
5	6	O	-0.705005	-1.886349	-0.210130
6	1	O	2.041308	-1.144465	2.220566
7	1	O	0.891465	-3.016592	1.428095
8	1	O	-0.160899	-0.167686	2.160644
9	1	O	-0.143481	0.078072	-0.849344
10	1	O	-1.129660	-2.376472	0.684178
11	8	O	0.567680	-2.434898	-0.513063
12	8	O	2.627249	-3.007984	0.333539
13	6	O	2.574294	-4.414743	0.041931
14	1	O	1.980403	-4.576148	-0.864457
15	1	O	2.078098	-4.934929	0.876358
16	6	O	3.998042	-4.908613	-0.138904
17	1	O	4.585903	-4.745848	0.769469
18	1	O	3.995818	-5.980037	-0.365396
19	1	O	4.485243	-4.381212	-0.964243
20	8	O	2.602772	-0.258379	0.453586
21	8	O	0.955072	1.208902	1.088267
22	5	O	2.211195	1.062864	0.527266
23	6	O	3.080261	2.248260	0.035046
24	6	O	2.594005	3.568919	0.077717
25	6	O	4.378498	2.029782	-0.464473
26	6	O	3.377896	4.636563	-0.363205
27	1	O	1.593808	3.754647	0.459395
28	6	O	5.165250	3.094479	-0.907197
29	1	O	4.767667	1.016172	-0.504308
30	6	O	4.665071	4.399649	-0.856312
31	1	O	2.988500	5.650070	-0.323814
32	1	O	6.165032	2.909655	-1.290168
33	1	O	5.276459	5.229722	-1.199900
34	6	O	-1.646602	-2.103094	-1.388512
35	1	O	-1.893367	-3.161851	-1.505611
36	1	O	-1.170396	-1.753390	-2.312174
37	8	O	-2.869622	-1.389788	-1.182874
38	8	O	-1.842648	0.189656	0.316512
39	5	O	-2.947546	-0.300475	-0.346933
40	6	O	-4.330371	0.391912	-0.130009
41	6	O	-4.448062	1.533141	0.686077
42	6	O	-5.494709	-0.104813	-0.746176
43	6	O	-5.682594	2.155630	0.881158
44	1	O	-3.560323	1.933335	1.167612
45	6	O	-6.731898	0.513175	-0.554454
46	1	O	-5.423213	-0.983514	-1.380883
47	6	O	-6.827354	1.645481	0.260770
48	1	O	-5.753495	3.036355	1.513600
49	1	O	-7.619630	0.115279	-1.038554
50	1	O	-7.789119	2.128600	0.411014

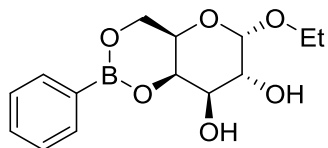


Ethyl β -D-mannofuranoside (bis-boronate)

Energy: -1276.69845028

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.282317	1.338788	0.292408
2	6	0	-1.727749	2.433802	0.479721
3	6	0	-1.819725	1.250520	1.502201
4	6	0	-0.507548	0.447246	1.263109
5	1	0	0.901294	2.033255	0.887958
6	1	0	-1.429386	3.355665	1.018470
7	1	0	-1.950962	1.610102	2.526075
8	1	0	0.065875	0.208707	2.161811
9	8	0	-0.706262	2.069934	-0.433188
10	8	0	-2.865313	2.665441	-0.278292
11	6	0	-3.918973	3.335170	0.421399
12	1	0	-4.287955	2.698581	1.237248
13	1	0	-3.530804	4.268202	0.860581
14	6	0	-5.028968	3.628863	-0.572384
15	1	0	-5.855317	4.143435	-0.070866
16	1	0	-4.662417	4.264751	-1.383674
17	1	0	-5.410154	2.700088	-1.006550
18	8	0	-2.877649	0.347343	1.188815
19	8	0	-0.949334	-0.776136	0.660454
20	6	0	1.183125	0.623734	-0.704889
21	1	0	0.605570	-0.148606	-1.220006
22	6	0	1.894351	1.578316	-1.701055
23	1	0	1.552081	1.442288	-2.729251
24	1	0	1.774438	2.631557	-1.427192
25	8	0	3.289318	1.229142	-1.615416
26	5	0	-2.327716	-0.797424	0.648934
27	8	0	2.256511	-0.013027	0.014783
28	5	0	3.450692	0.337016	-0.582461
29	6	0	-3.164792	-1.989568	0.117342
30	6	0	-4.571429	-1.937557	0.106196
31	6	0	-2.536762	-3.155326	-0.360795
32	6	0	-5.326330	-3.011943	-0.367416
33	1	0	-5.072529	-1.045661	0.471762
34	6	0	-3.287336	-4.232265	-0.835746
35	1	0	-1.451845	-3.213955	-0.357367
36	6	0	-4.683995	-4.161135	-0.839357
37	1	0	-6.411333	-2.955530	-0.369941
38	1	0	-2.787107	-5.124533	-1.201712
39	1	0	-5.269936	-4.998382	-1.208778
40	6	0	4.828058	-0.218582	-0.128563
41	6	0	4.919628	-1.169182	0.905762
42	6	0	6.018556	0.214532	-0.742576
43	6	0	6.157131	-1.669815	1.314711
44	1	0	4.010588	-1.517597	1.388297
45	6	0	7.258439	-0.282812	-0.337066
46	1	0	5.966217	0.946194	-1.544063
47	6	0	7.328697	-1.226243	0.693017
48	1	0	6.209922	-2.403962	2.113938
49	1	0	8.167719	0.061836	-0.821752
50	1	0	8.292819	-1.615235	1.009289

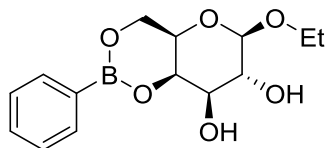


Ethyl α -D-galactopyranoside (mono-boronate 1,3-diol)

Energy: -981.961495900

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
X	Y	Z			
1	6	0	1.387438	-1.210929	0.767547
2	6	0	0.892749	0.130924	1.325359
3	6	0	1.796854	1.287791	0.885509
4	6	0	2.032281	1.233092	-0.627872
5	6	0	2.579990	-0.141246	-1.025603
6	8	0	1.638330	-1.145356	-0.642298
7	6	0	0.341177	-2.293127	0.993673
8	8	0	-0.438483	0.432429	0.874254
9	8	0	1.255571	2.551394	1.262648
10	8	0	2.924485	2.244045	-1.059292
11	8	0	3.828844	-0.334087	-0.424447
12	5	0	-1.318628	-0.570818	0.521633
13	8	0	-0.967750	-1.891940	0.587488
14	6	0	-2.756973	-0.189267	0.043447
15	6	0	-3.661144	-1.185412	-0.372003
16	6	0	-4.948699	-0.858513	-0.801350
17	6	0	-5.360281	0.477828	-0.821122
18	6	0	-4.479452	1.483098	-0.410483
19	6	0	-3.192758	1.148741	0.016200
20	6	0	4.595784	-1.397110	-0.985790
21	1	0	2.309906	-1.489617	1.295116
22	1	0	0.873065	0.082967	2.422200
23	1	0	2.762011	1.206272	1.394347
24	1	0	1.062469	1.336279	-1.136991
25	1	0	2.652845	-0.231435	-2.116550
26	1	0	0.603411	-3.185112	0.418532
27	1	0	0.312807	-2.558214	2.058047
28	1	0	0.305548	2.523335	1.068037
29	1	0	2.646164	3.068300	-0.633248
30	1	0	-3.344783	-2.224381	-0.357504
31	1	0	-5.630840	-1.642073	-1.119713
32	1	0	-6.362221	0.734492	-1.154316
33	1	0	-4.795811	2.522491	-0.423078
34	1	0	-2.515244	1.935719	0.335511
35	1	0	4.777071	-1.221327	-2.054700
36	1	0	4.096700	-2.365505	-0.859145
37	1	0	5.550281	-1.405212	-0.456620

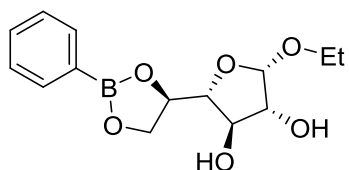


Ethyl β -D-galactopyranoside (mono-boronate 1,3-diol)

Energy: -981.959087566

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.352180	0.879154	-1.439188
2	6	0	0.869707	-0.581193	-1.505191
3	6	0	1.917540	-1.496612	-0.870775
4	6	0	2.246718	-1.023572	0.542988
5	6	0	2.683853	0.442865	0.501275
6	8	0	1.669258	1.249164	-0.094660
7	6	0	0.254920	1.816490	-1.924933
8	8	0	-0.378279	-0.725173	-0.832885
9	8	0	1.466026	-2.836662	-0.897743
10	8	0	3.292167	-1.864548	1.025977
11	8	0	2.889285	0.861003	1.810400
12	6	0	3.487204	2.152421	1.943594
13	5	0	-1.276001	0.314316	-0.770560
14	8	0	-1.006828	1.543246	-1.321464
15	6	0	-2.648371	0.083144	-0.059894
16	6	0	-3.583725	1.126686	0.071469
17	6	0	-4.811188	0.920062	0.704241
18	6	0	-5.127497	-0.341616	1.218194
19	6	0	-4.212546	-1.392216	1.096688
20	6	0	-2.986209	-1.179302	0.463460
21	1	0	2.238764	1.002495	-2.083358
22	1	0	0.738979	-0.877548	-2.554822
23	1	0	2.835456	-1.400136	-1.477258
24	1	0	1.355050	-1.102146	1.176832
25	1	0	3.616843	0.547868	-0.087017
26	1	0	0.520417	2.849995	-1.684378
27	1	0	0.155552	1.725993	-3.014152
28	1	0	2.079531	-3.356183	-0.357816
29	1	0	3.480086	-1.613953	1.940969
30	1	0	2.818485	2.933842	1.570293
31	1	0	4.443244	2.194657	1.403427
32	1	0	3.666025	2.299797	3.009745
33	1	0	-3.340669	2.107648	-0.327127
34	1	0	-5.520128	1.738437	0.797031
35	1	0	-6.082520	-0.505335	1.710410
36	1	0	-4.456089	-2.373998	1.493793
37	1	0	-2.277569	-1.997120	0.367661

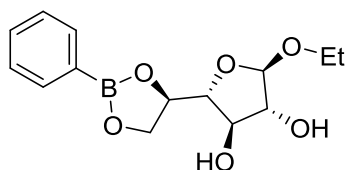


Ethyl α -D-galactofuranoside (mono-boronate)

Energy: -981.955387542

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
X	Y	Z			
1	6	0	-1.447662	-0.388293	-0.526169
2	6	0	-2.725253	-1.154088	-0.150111
3	6	0	-3.834363	-0.281249	-0.761336
4	6	0	-3.256518	1.125192	-0.562573
5	8	0	-1.863011	0.982752	-0.739177
6	6	0	-0.346235	-0.446796	0.523566
7	8	0	-2.668844	-2.476779	-0.663289
8	8	0	-5.116771	-0.488196	-0.209086
9	8	0	-3.608506	1.520262	0.748757
10	8	0	0.817796	0.271621	0.075941
11	6	0	0.180041	-1.882351	0.800809
12	8	0	1.613005	-1.754316	0.802895
13	5	0	1.930019	-0.507046	0.314284
14	6	0	3.384439	-0.025574	0.060319
15	6	0	3.641553	1.271952	-0.421606
16	6	0	4.948172	1.707645	-0.650076
17	6	0	6.023627	0.849828	-0.398073
18	6	0	5.788480	-0.442981	0.080967
19	6	0	4.480063	-0.874442	0.306803
20	6	0	-3.239459	2.860171	1.080667
21	1	0	-1.057077	-0.775747	-1.475702
22	1	0	-2.860095	-1.173397	0.942116
23	1	0	-3.902351	-0.504024	-1.831542
24	1	0	-3.600707	1.879371	-1.281369
25	1	0	-0.706990	0.038305	1.439482
26	1	0	-3.502043	-2.919976	-0.450056
27	1	0	-5.166228	0.046446	0.599603
28	1	0	-0.113999	-2.590805	0.019907
29	1	0	-0.146707	-2.271578	1.768499
30	1	0	2.806987	1.939384	-0.617952
31	1	0	5.129481	2.711890	-1.023180
32	1	0	7.041340	1.187388	-0.574874
33	1	0	6.623056	-1.110647	0.276571
34	1	0	4.299438	-1.879460	0.678059
35	1	0	-3.710337	3.573124	0.390178
36	1	0	-2.152166	2.984629	1.048112
37	1	0	-3.602364	3.043502	2.093281

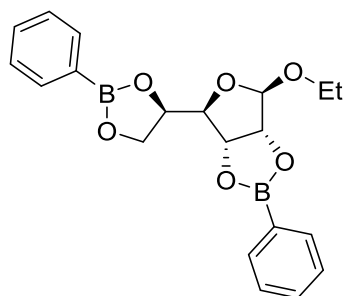


Ethyl β -D-galactofuranoside (mono-boronate)

Energy: -981.951826831

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.506916	-0.356730	0.063922
2	6	0	2.747017	-1.250973	-0.068013
3	6	0	3.874210	-0.262979	0.228446
4	6	0	3.320622	1.077210	-0.292041
5	8	0	1.934731	0.864888	-0.558082
6	6	0	0.262784	-0.863662	-0.645732
7	8	0	2.684810	-2.359778	0.814122
8	8	0	5.074250	-0.704623	-0.394229
9	8	0	3.537683	2.051392	0.695848
10	8	0	-0.832340	0.053149	-0.459764
11	6	0	-0.281304	-2.210335	-0.099256
12	8	0	-1.707627	-2.024035	-0.033124
13	5	0	-1.965420	-0.680020	-0.178232
14	6	0	-3.379924	-0.052935	-0.042747
15	6	0	-3.579275	1.326555	-0.240566
16	6	0	-4.849471	1.893705	-0.121055
17	6	0	-5.946275	1.086983	0.198470
18	6	0	-5.768538	-0.285803	0.398444
19	6	0	-4.496166	-0.848045	0.278946
20	6	0	3.114955	3.363290	0.320736
21	1	0	1.274278	-0.191588	1.126817
22	1	0	2.846445	-1.587553	-1.111690
23	1	0	4.002168	-0.184696	1.315703
24	1	0	3.782322	1.389460	-1.239637
25	1	0	0.473229	-0.916075	-1.721896
26	1	0	3.487781	-2.885859	0.698946
27	1	0	5.819616	-0.203184	-0.038772
28	1	0	0.095904	-2.435568	0.902503
29	1	0	-0.057352	-3.054597	-0.755238
30	1	0	-2.728388	1.954394	-0.490243
31	1	0	-4.986010	2.960330	-0.276865
32	1	0	-6.935904	1.526289	0.291224
33	1	0	-6.619725	-0.913825	0.646815
34	1	0	-4.360289	-1.914629	0.435402
35	1	0	2.034032	3.392884	0.150454
36	1	0	3.636862	3.696195	-0.587936
37	1	0	3.376770	4.022481	1.150060

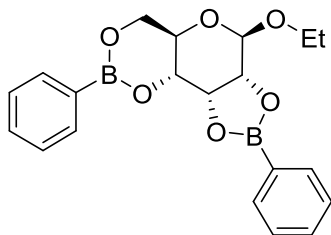


Ethyl β -D-allofuranoside (bis-boronate)

Energy: -1237.38328141

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.794703	0.422683	0.703633
2	6	0	-0.032996	0.874012	-0.509891
3	8	0	0.751967	1.902647	-1.146554
4	6	0	1.498792	2.595803	-0.181924
5	6	0	1.832601	1.565350	0.916943
6	6	0	-1.423707	1.409030	-0.149200
7	6	0	-2.231772	1.909069	-1.376623
8	8	0	-3.460206	1.157552	-1.346302
9	8	0	1.588655	-0.734159	0.397478
10	8	0	0.707854	3.656562	0.336900
11	8	0	3.109540	0.957051	0.694390
12	8	0	-2.212098	0.330119	0.392694
13	5	0	2.917687	-0.374838	0.382070
14	5	0	-3.390032	0.243273	-0.323376
15	6	0	-4.512484	-0.780688	-0.001965
16	6	0	-4.386965	-1.679537	1.074117
17	6	0	-5.395355	-2.600821	1.363043
18	6	0	-6.551350	-2.638606	0.576895
19	6	0	-6.694860	-1.753848	-0.496689
20	6	0	-5.683571	-0.834512	-0.781459
21	6	0	4.074422	-1.354777	0.055232
22	6	0	5.414157	-0.922371	0.072306
23	6	0	6.456703	-1.801878	-0.224571
24	6	0	6.175258	-3.133762	-0.545040
25	6	0	4.850843	-3.582513	-0.566648
26	6	0	3.811575	-2.699528	-0.268423
27	6	0	1.465601	4.731217	0.882052
28	1	0	0.168939	0.198635	1.569524
29	1	0	-0.134590	0.053766	-1.226740
30	1	0	2.397389	2.992800	-0.669847
31	1	0	1.818826	2.015549	1.912330
32	1	0	-1.335248	2.189086	0.613018
33	1	0	-1.716388	1.712329	-2.321920
34	1	0	-2.462729	2.975200	-1.318921
35	1	0	-3.489658	-1.652812	1.686181
36	1	0	-5.282091	-3.287611	2.197299
37	1	0	-7.337426	-3.354939	0.800083
38	1	0	-7.592262	-1.782288	-1.108539
39	1	0	-5.797179	-0.148782	-1.616522
40	1	0	5.635638	0.112050	0.320115
41	1	0	7.485203	-1.452207	-0.207517
42	1	0	6.985380	-3.819695	-0.777334
43	1	0	4.631025	-4.616899	-0.815659
44	1	0	2.783571	-3.050682	-0.285902
45	1	0	2.137782	5.161858	0.126525
46	1	0	2.061784	4.418489	1.750838
47	1	0	0.748485	5.489873	1.199956

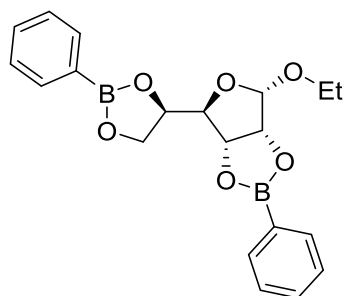


Ethyl β -D-allopyranoside (bis-boronate)

Energy: -1237.38005772

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.701012	1.270738	-0.902173
2	6	0	0.509946	1.972584	0.440081
3	8	0	-0.465874	2.993296	0.262456
4	6	0	-1.836543	1.531032	-1.189800
5	6	0	-0.593228	0.624139	-1.376557
6	8	0	1.760037	0.322646	-0.857563
7	6	0	3.989303	-0.500036	0.022902
8	6	0	1.826638	2.598397	0.879350
9	8	0	-2.664708	3.486986	-0.145476
10	8	0	-2.899241	0.578938	-0.999787
11	8	0	-0.939501	-0.559375	-0.632659
12	5	0	-2.318771	-0.599524	-0.564958
13	6	0	-3.124111	-1.820225	-0.052003
14	8	0	2.868729	1.619033	0.843409
15	5	0	2.817314	0.531912	0.002055
16	6	0	3.965474	-1.638632	-0.804679
17	6	0	5.011440	-2.563450	-0.788839
18	6	0	6.105834	-2.364941	0.058804
19	6	0	6.148925	-1.240235	0.888839
20	6	0	5.099900	-0.319060	0.868840
21	6	0	-2.468722	-3.005677	0.332889
22	6	0	-3.191411	-4.107360	0.793999
23	6	0	-4.586152	-4.042071	0.875008
24	6	0	-5.255199	-2.873959	0.495236
25	6	0	-4.528698	-1.773682	0.036936
26	6	0	-2.938635	4.275237	1.014830
27	1	0	0.952644	2.049099	-1.638509
28	1	0	0.178685	1.245248	1.197845
29	1	0	-2.052293	2.148393	-2.064786
30	1	0	-0.485326	0.333205	-2.429250
31	1	0	1.762541	2.979520	1.902017
32	1	0	2.083597	3.432160	0.214436
33	1	0	3.115689	-1.795849	-1.462764
34	1	0	4.974780	-3.436860	-1.434240
35	1	0	6.921139	-3.083326	0.072502
36	1	0	6.998013	-1.083633	1.548596
37	1	0	5.135815	0.553266	1.515245
38	1	0	-1.385474	-3.058681	0.267807
39	1	0	-2.671262	-5.014707	1.087971
40	1	0	-5.150241	-4.899381	1.232254
41	1	0	-6.338732	-2.823375	0.556501
42	1	0	-5.049966	-0.867255	-0.258461
43	1	0	-2.045491	4.813330	1.347720
44	1	0	-3.315908	3.644232	1.831209
45	1	0	-3.710861	4.988504	0.723281
46	6	0	-1.775518	2.447066	0.054525
47	1	0	-2.047145	1.862780	0.952979

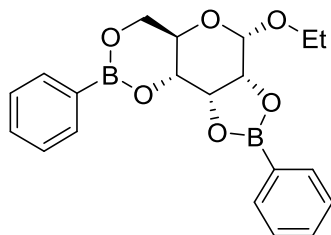


Ethyl α -D-allofuranoside (bis-boronate)

Energy: -1237.37915829

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.728600	0.954129	1.129407
2	6	0	-0.174418	1.706792	0.134450
3	8	0	0.453805	2.995443	-0.040277
4	6	0	1.847581	2.838134	0.050216
5	6	0	2.022923	1.809728	1.206953
6	6	0	-1.596161	1.975650	0.617066
7	6	0	-2.483562	2.707588	-0.427719
8	8	0	-3.522948	1.768536	-0.758626
9	8	0	1.175354	-0.320316	0.649519
10	8	0	2.334663	2.347188	-1.174579
11	8	0	3.095720	0.894162	1.008304
12	8	0	-2.261227	0.722925	0.847546
13	5	0	2.552750	-0.313167	0.602121
14	5	0	-3.358754	0.642663	0.012185
15	6	0	-4.302319	-0.588468	-0.044347
16	6	0	-4.064455	-1.720150	0.758446
17	6	0	-4.912503	-2.827944	0.707746
18	6	0	-6.016639	-2.822303	-0.150516
19	6	0	-6.269295	-1.707501	-0.956430
20	6	0	-5.418454	-0.602103	-0.902168
21	6	0	3.405762	-1.534824	0.170697
22	6	0	4.812154	-1.473121	0.171021
23	6	0	5.580443	-2.573351	-0.213774
24	6	0	4.951583	-3.758559	-0.608365
25	6	0	3.555398	-3.839814	-0.615066
26	6	0	2.791581	-2.737524	-0.227357
27	6	0	3.673712	2.726201	-1.484551
28	1	0	0.233170	0.805503	2.093003
29	1	0	-0.196226	1.162594	-0.818487
30	1	0	2.275342	3.825120	0.266487
31	1	0	2.154617	2.324685	2.162156
32	1	0	-1.551444	2.525019	1.564951
33	1	0	-1.930297	2.966807	-1.334563
34	1	0	-2.942088	3.614155	-0.022735
35	1	0	-3.205994	-1.728137	1.424323
36	1	0	-4.714436	-3.693692	1.333606
37	1	0	-6.677697	-3.683813	-0.191631
38	1	0	-7.126400	-1.702011	-1.624132
39	1	0	-5.615629	0.262609	-1.529709
40	1	0	5.303751	-0.554238	0.478737
41	1	0	6.665030	-2.509321	-0.206540
42	1	0	5.547532	-4.616051	-0.908963
43	1	0	3.065616	-4.760001	-0.921150
44	1	0	1.707176	-2.803392	-0.232572
45	1	0	4.389832	2.292148	-0.778244
46	1	0	3.776406	3.821061	-1.488917
47	1	0	3.877239	2.344606	-2.486483

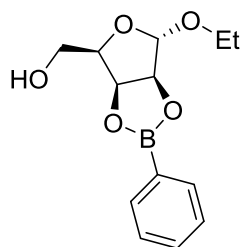


Ethyl α -D-allopyranoside (bis-boronate)

Energy: -1237.37842059

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.804016	1.265853	1.060400
2	6	0	-0.654956	2.071077	-0.224491
3	8	0	0.255579	3.147265	0.027110
4	6	0	1.596260	2.696958	0.218207
5	6	0	1.690343	1.713935	1.427445
6	6	0	0.529915	0.693178	1.515397
7	8	0	-1.788343	0.247302	0.927827
8	6	0	-3.951181	-0.655460	-0.035537
9	6	0	-2.007016	2.644484	-0.623721
10	8	0	2.103172	2.068166	-0.920219
11	8	0	2.837301	0.869953	1.292587
12	8	0	1.009066	-0.398447	0.711795
13	6	0	2.356346	2.943169	-2.018428
14	5	0	2.388689	-0.305607	0.707469
15	6	0	3.328937	-1.408431	0.157720
16	8	0	-2.982679	1.598486	-0.670016
17	5	0	-2.854946	0.451304	0.078750
18	6	0	-3.844675	-1.856254	0.691618
19	6	0	-4.822969	-2.847735	0.593612
20	6	0	-5.931301	-2.655117	-0.237080
21	6	0	-6.055851	-1.469495	-0.968259
22	6	0	-5.073908	-0.482014	-0.866829
23	6	0	2.809888	-2.628543	-0.315537
24	6	0	3.654382	-3.624042	-0.810450
25	6	0	5.037093	-3.415865	-0.837509
26	6	0	5.571699	-2.210795	-0.370197
27	6	0	4.723192	-1.217619	0.122111
28	1	0	-1.124142	1.964913	1.848790
29	1	0	-0.270947	1.427731	-1.025461
30	1	0	2.158313	3.615162	0.434098
31	1	0	1.780437	2.307651	2.340945
32	1	0	0.427186	0.327105	2.545696
33	1	0	-1.966556	3.105673	-1.614249
34	1	0	-2.322875	3.406408	0.099745
35	1	0	3.060754	3.734688	-1.727698
36	1	0	1.432538	3.401001	-2.389604
37	1	0	2.803835	2.331015	-2.802814
38	1	0	-2.983698	-2.009228	1.336002
39	1	0	-4.722736	-3.768478	1.161897
40	1	0	-6.693984	-3.425398	-0.314585
41	1	0	-6.915690	-1.317354	-1.615037
42	1	0	-5.172599	0.437281	-1.437128
43	1	0	1.736048	-2.792502	-0.293919
44	1	0	3.237974	-4.559808	-1.172912
45	1	0	5.695991	-4.190237	-1.221095
46	1	0	6.645809	-2.048177	-0.390535
47	1	0	5.139779	-0.281418	0.483268

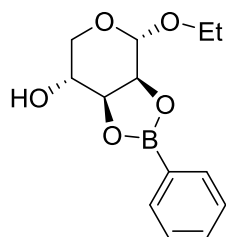


Ethyl α -D-lyxofuranoside (mono-boronate)

Energy: -867.421625926

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.107005	1.040310	0.374485
2	6	0	-1.085024	0.367676	1.306559
3	6	0	-1.111647	-1.131587	0.878669
4	6	0	-2.108139	-1.176154	-0.291662
5	8	0	-2.195309	0.157319	-0.767608
6	6	0	-1.759846	2.432499	-0.129932
7	5	0	0.978477	-0.268158	0.542387
8	8	0	0.264626	0.793073	1.056464
9	8	0	0.220234	-1.415655	0.438113
10	8	0	-3.327194	-1.651513	0.223528
11	6	0	-4.363261	-1.774972	-0.750069
12	8	0	-2.795200	2.960656	-0.952684
13	6	0	2.473143	-0.185242	0.136903
14	6	0	3.198522	1.011511	0.291654
15	6	0	4.544251	1.087986	-0.071425
16	6	0	5.189432	-0.035720	-0.597611
17	6	0	4.486167	-1.233812	-0.758493
18	6	0	3.140706	-1.305630	-0.393483
19	1	0	-3.083746	1.071034	0.876151
20	1	0	-1.313188	0.542319	2.360889
21	1	0	-1.395219	-1.834601	1.663801
22	1	0	-1.764218	-1.791045	-1.132083
23	1	0	-0.802529	2.403159	-0.662760
24	1	0	-1.659371	3.116058	0.718157
25	1	0	-4.051630	-2.441209	-1.566908
26	1	0	-4.638302	-0.799313	-1.164969
27	1	0	-5.221404	-2.210855	-0.235931
28	1	0	-2.894146	2.371038	-1.712891
29	1	0	2.700483	1.886116	0.700995
30	1	0	5.089565	2.019159	0.054463
31	1	0	6.236815	0.022042	-0.881148
32	1	0	4.986457	-2.107480	-1.166823
33	1	0	2.597000	-2.237871	-0.518946

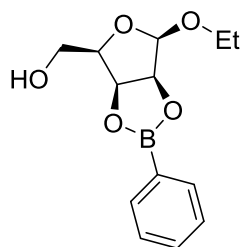


Ethyl α -D-lyxopyranoside (mono-boronate)

Energy: -867.417730158

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
X	Y	Z			
1	6	0	2.880837	1.086176	0.911824
2	6	0	1.550135	1.685402	0.470158
3	6	0	1.018622	0.941133	-0.761076
4	6	0	1.171244	-0.595048	-0.685353
5	6	0	2.352115	-1.112432	0.149458
6	8	0	2.676008	-0.290227	1.252140
7	8	0	-0.088527	-1.031034	-0.137251
8	8	0	3.429006	-1.244470	-0.752261
9	6	0	4.575806	-1.890038	-0.200814
10	8	0	-0.413678	1.127467	-0.852196
11	8	0	1.755074	3.068343	0.201869
12	5	0	-1.006048	-0.026672	-0.371737
13	6	0	-2.529557	-0.178908	-0.122928
14	6	0	-3.413996	0.890591	-0.360165
15	6	0	-4.785389	0.751653	-0.139318
16	6	0	-5.296908	-0.463799	0.326554
17	6	0	-4.434669	-1.537942	0.568771
18	6	0	-3.064404	-1.394879	0.343979
19	1	0	3.239894	1.578940	1.816864
20	1	0	3.639531	1.190494	0.126154
21	1	0	0.833373	1.555682	1.293313
22	1	0	1.487285	1.356002	-1.657735
23	1	0	1.269451	-1.023064	-1.688648
24	1	0	2.092442	-2.081902	0.594068
25	1	0	5.303228	-1.971341	-1.010205
26	1	0	4.318599	-2.895569	0.160785
27	1	0	5.004225	-1.311906	0.624889
28	1	0	0.902284	3.469265	-0.014617
29	1	0	-3.020045	1.835959	-0.723093
30	1	0	-5.454532	1.586293	-0.328992
31	1	0	-6.364011	-0.573618	0.499694
32	1	0	-4.830914	-2.482741	0.930254
33	1	0	-2.396649	-2.231226	0.531005

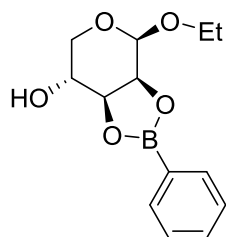


Ethyl β -D-lyxofuranoside (mono-boronate)

Energy: -867.412787227

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
X	Y	Z			
1	6	0	2.310137	-1.140967	0.379205
2	6	0	1.209637	-0.788837	1.396718
3	6	0	1.193428	0.772032	1.406305
4	6	0	2.266851	1.154139	0.359357
5	8	0	2.392664	0.001306	-0.485173
6	6	0	2.081248	-2.379448	-0.474025
7	5	0	-0.831048	-0.012919	0.711225
8	8	0	-0.100320	-1.160674	0.946071
9	8	0	-0.124470	1.132040	1.003404
10	8	0	3.185420	-2.626792	-1.337686
11	8	0	1.913489	2.270621	-0.363257
12	6	0	2.932257	2.750982	-1.241737
13	6	0	-2.294352	-0.013332	0.197930
14	6	0	-2.985681	-1.219786	-0.022181
15	6	0	-4.302627	-1.218902	-0.485117
16	6	0	-4.952204	-0.006198	-0.736729
17	6	0	-4.282063	1.202788	-0.523878
18	6	0	-2.965461	1.197131	-0.060122
19	1	0	3.265317	-1.253244	0.919650
20	1	0	1.386428	-1.252640	2.371096
21	1	0	1.405432	1.229534	2.376305
22	1	0	3.238308	1.308531	0.870118
23	1	0	1.148437	-2.267027	-1.038034
24	1	0	1.989450	-3.258171	0.171024
25	1	0	3.285193	-1.855646	-1.912874
26	1	0	3.126974	2.036047	-2.047775
27	1	0	3.863922	2.945405	-0.691535
28	1	0	2.558119	3.685693	-1.661953
29	1	0	-2.483716	-2.163652	0.172204
30	1	0	-4.822102	-2.158775	-0.650025
31	1	0	-5.977161	-0.003399	-1.097692
32	1	0	-4.785424	2.145393	-0.720154
33	1	0	-2.445209	2.136928	0.102288

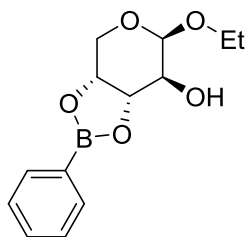


Ethyl β -D-lyxopyranoside (mono-boronate)

Energy: -867.410896630

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.952010	1.235937	-0.838268
2	6	0	-1.592457	1.835395	-0.482920
3	6	0	-1.052384	1.239961	0.828546
4	6	0	-1.272017	-0.284839	0.967664
5	6	0	-2.573914	-0.776543	0.328133
6	8	0	-2.826660	-0.179099	-0.938384
7	8	0	-0.081181	-0.841926	0.391072
8	8	0	0.387506	1.362386	0.842193
9	8	0	-1.745379	3.247973	-0.394147
10	8	0	-2.526993	-2.151426	0.198966
11	6	0	-3.764644	-2.752004	-0.184928
12	5	0	0.894066	0.129606	0.458481
13	6	0	2.388990	-0.126763	0.135701
14	6	0	3.335222	0.914146	0.194254
15	6	0	4.679819	0.680179	-0.099128
16	6	0	5.101237	-0.603880	-0.459273
17	6	0	4.176278	-1.650978	-0.523243
18	6	0	2.833112	-1.412853	-0.226856
19	1	0	-3.285838	1.599704	-1.811734
20	1	0	-3.708053	1.514758	-0.086143
21	1	0	-0.894865	1.574003	-1.290351
22	1	0	-1.463708	1.802200	1.672477
23	1	0	-1.298523	-0.576100	2.026303
24	1	0	-3.402720	-0.477703	1.006008
25	1	0	-0.872360	3.645548	-0.273681
26	1	0	-4.051796	-2.453476	-1.197601
27	1	0	-4.564962	-2.480044	0.518673
28	1	0	-3.603134	-3.830440	-0.148923
29	1	0	3.010943	1.912877	0.473867
30	1	0	5.397768	1.494070	-0.048441
31	1	0	6.147237	-0.787858	-0.689183
32	1	0	4.502845	-2.648744	-0.802763
33	1	0	2.115105	-2.226638	-0.276601

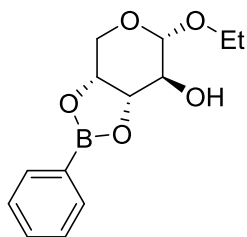


Ethyl β -D-arabinopyranoside (mono-boronate)

Energy: -867.417460806

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.994691	0.532489	0.846508
2	6	0	-0.886843	-1.009543	0.947033
3	6	0	-2.013040	-1.790082	0.285154
4	8	0	-2.482031	-1.215451	-0.938521
5	6	0	-2.881757	0.132966	-0.820801
6	6	0	-1.702685	1.032742	-0.429407
7	8	0	0.384038	0.954932	0.826436
8	8	0	0.402821	-1.293355	0.364305
9	5	0	1.143783	-0.129586	0.436322
10	8	0	-3.889542	0.331426	0.152036
11	8	0	-2.112533	2.386142	-0.322471
12	6	0	-5.169874	-0.190473	-0.206989
13	6	0	2.659431	-0.048538	0.115589
14	6	0	3.390363	-1.202543	-0.225379
15	6	0	4.754838	-1.130230	-0.511492
16	6	0	5.413838	0.102262	-0.458406
17	6	0	4.705264	1.259776	-0.120527
18	6	0	3.340477	1.182947	0.162852
19	1	0	-1.479511	0.964422	1.725805
20	1	0	-0.841095	-1.314648	2.001913
21	1	0	-1.663221	-2.791975	0.028072
22	1	0	-2.845164	-1.876833	0.995379
23	1	0	-3.257328	0.408436	-1.814476
24	1	0	-0.983466	0.996511	-1.252550
25	1	0	-2.919272	2.398840	0.214696
26	1	0	-5.131122	-1.276768	-0.344211
27	1	0	-5.533005	0.277171	-1.131927
28	1	0	-5.847991	0.052210	0.612963
29	1	0	2.880506	-2.161164	-0.266354
30	1	0	5.304320	-2.029943	-0.774309
31	1	0	6.476121	0.160479	-0.679923
32	1	0	5.216248	2.217692	-0.079366
33	1	0	2.791102	2.083305	0.423581

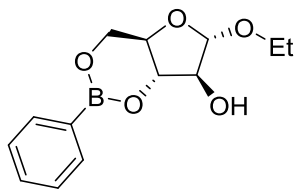


Ethyl α -D-arabinopyranoside (mono-boronate)

Energy: -867.416383276

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
X	Y	Z			
1	6	0	0.918664	0.426270	-1.260950
2	6	0	0.776556	-1.120047	-1.262869
3	6	0	1.950513	-1.884062	-0.658150
4	8	0	2.513356	-1.239127	0.477042
5	6	0	2.996349	0.055474	0.144455
6	6	0	1.815093	0.985003	-0.146382
7	8	0	-0.435190	0.881928	-1.073736
8	8	0	-0.450202	-1.350562	-0.542897
9	5	0	-1.164652	-0.169358	-0.556876
10	8	0	3.683638	0.591843	1.227877
11	8	0	2.260460	2.270327	-0.555823
12	6	0	-2.624923	-0.037202	-0.050245
13	6	0	-3.335777	-1.161615	0.410774
14	6	0	-4.650463	-1.043682	0.865242
15	6	0	-5.278790	0.205803	0.864637
16	6	0	-4.589369	1.334550	0.410060
17	6	0	-3.274387	1.211986	-0.042409
18	6	0	4.919726	-0.056199	1.534964
19	1	0	1.284812	0.806330	-2.219019
20	1	0	0.626109	-1.481449	-2.289592
21	1	0	1.615172	-2.869032	-0.326563
22	1	0	2.723667	-2.019161	-1.432964
23	1	0	3.665709	-0.022308	-0.735964
24	1	0	1.229913	1.046173	0.781324
25	1	0	2.801894	2.632275	0.159837
26	1	0	-2.849525	-2.133262	0.412181
27	1	0	-5.184975	-1.921184	1.218451
28	1	0	-6.302306	0.299589	1.217495
29	1	0	-5.076467	2.305712	0.409717
30	1	0	-2.739821	2.090056	-0.394099
31	1	0	5.591130	-0.043902	0.665060
32	1	0	4.751161	-1.088874	1.854957
33	1	0	5.371145	0.512876	2.349091

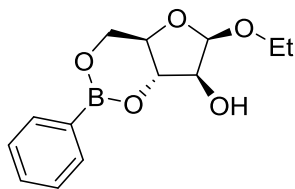


Ethyl α -D-arabinofuranoside (mono-boronate 1,3-diol)

Energy: -867.408831647

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.435589	-0.996458	0.045291
2	6	0	-1.026237	0.336310	0.651692
3	6	0	-2.159851	1.241248	0.177457
4	6	0	-3.355000	0.253694	0.130995
5	8	0	-2.821345	-1.068383	0.369153
6	6	0	-0.558139	-2.089826	0.620626
7	8	0	0.295392	0.694743	0.273175
8	8	0	-2.480951	2.317614	1.045781
9	8	0	-3.957516	0.352242	-1.126540
10	8	0	0.809781	-1.662384	0.468168
11	5	0	1.198200	-0.357847	0.255299
12	6	0	2.706505	-0.057993	-0.017501
13	6	0	3.159376	1.260739	-0.212627
14	6	0	4.506489	1.532489	-0.459515
15	6	0	5.430762	0.484572	-0.514396
16	6	0	5.002168	-0.832685	-0.322090
17	6	0	3.653704	-1.097982	-0.076457
18	6	0	-5.167832	-0.394697	-1.253133
19	1	0	-1.298038	-0.963399	-1.047587
20	1	0	-1.083798	0.269012	1.747481
21	1	0	-1.960626	1.597463	-0.841175
22	1	0	-4.081039	0.446107	0.930296
23	1	0	-0.772712	-2.245120	1.684145
24	1	0	-0.661289	-3.043572	0.096418
25	1	0	-1.794819	2.993475	0.969204
26	1	0	2.444599	2.077681	-0.170428
27	1	0	4.836509	2.556993	-0.608455
28	1	0	6.479828	0.693489	-0.705973
29	1	0	5.718187	-1.648916	-0.363922
30	1	0	3.323462	-2.122008	0.072337
31	1	0	-5.905026	-0.069606	-0.505696
32	1	0	-4.983411	-1.468372	-1.139854
33	1	0	-5.553843	-0.191117	-2.253238

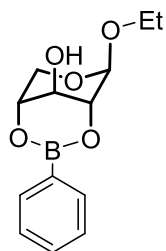


Ethyl β -D-arabinofuranoside (mono-boronate 1,3-diol)

Energy: -867.401038243

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.299672	1.190096	-0.596621
2	6	0	1.095715	-0.162242	0.064212
3	6	0	2.201642	-0.954148	-0.612134
4	6	0	3.355109	0.094753	-0.520948
5	8	0	2.714920	1.369594	-0.622851
6	6	0	0.493299	2.225750	0.163563
7	8	0	-0.244913	-0.604099	-0.101509
8	8	0	2.584939	-2.169778	-0.001523
9	8	0	4.019476	0.058525	0.710919
10	8	0	-0.852276	1.712471	0.257729
11	5	0	-1.196960	0.391307	0.076528
12	6	0	5.223231	-0.707412	0.735090
13	6	0	-2.709472	0.002071	0.070581
14	6	0	-3.112202	-1.340435	-0.062107
15	6	0	-4.463485	-1.691941	-0.066732
16	6	0	-5.442145	-0.701525	0.062542
17	6	0	-5.063789	0.638184	0.195960
18	6	0	-3.710972	0.983142	0.199855
19	1	0	0.914820	1.143310	-1.628444
20	1	0	1.327094	-0.102549	1.136029
21	1	0	1.942560	-1.113592	-1.670445
22	1	0	4.079642	-0.000395	-1.341347
23	1	0	0.895787	2.378628	1.170789
24	1	0	0.438579	3.190182	-0.348036
25	1	0	1.840128	-2.783617	-0.049794
26	1	0	5.912318	-0.375344	-0.054955
27	1	0	5.021142	-1.777384	0.623571
28	1	0	5.681794	-0.521736	1.708041
29	1	0	-2.355224	-2.113222	-0.161597
30	1	0	-4.754531	-2.733754	-0.169820
31	1	0	-6.494510	-0.972496	0.059707
32	1	0	-5.822108	1.409792	0.297039
33	1	0	-3.419482	2.024182	0.304937

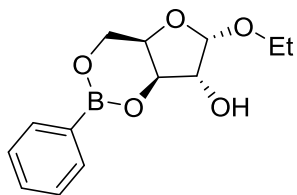


Ethyl β -D-xylopyranoside (mono-boronate 1,3 diol)

Energy: -867.421734359

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-1.677863	0.326922	-1.385199
2	6	0	-1.817211	-1.103231	-1.317461
3	6	0	-1.092688	-1.683313	-0.104398
4	6	0	-1.607937	-1.035441	1.194413
5	6	0	-1.335975	0.469871	1.038780
6	6	0	-2.037137	1.029630	-0.216905
7	6	0	2.375179	0.013141	0.082540
8	6	0	3.207427	-0.920690	-0.563323
9	8	0	0.316146	-1.437847	-0.215495
10	8	0	-2.962692	-1.350572	1.463053
11	8	0	0.068176	0.683253	0.897474
12	8	0	-3.431813	0.984986	0.041431
13	6	0	4.575579	-0.685970	-0.713184
14	5	0	0.845988	-0.257340	0.250394
15	6	0	5.139762	0.493458	-0.216847
16	6	0	4.330879	1.434251	0.428272
17	6	0	2.963213	1.193719	0.574487
18	6	0	-4.237662	1.648913	-0.937477
19	1	0	-2.876607	-1.387602	-1.286594
20	1	0	-1.375047	-1.478363	-2.242215
21	1	0	-1.238496	-2.767474	-0.076222
22	1	0	-1.019972	-1.415800	2.036734
23	1	0	-1.674756	1.027587	1.916068
24	1	0	-1.717680	2.061934	-0.404803
25	1	0	2.772298	-1.838199	-0.949181
26	1	0	-3.527340	-0.689466	1.027825
27	1	0	5.201482	-1.419074	-1.214746
28	1	0	6.204495	0.678195	-0.331686
29	1	0	4.766415	2.351340	0.815620
30	1	0	2.338173	1.926541	1.076924
31	1	0	-4.130279	1.181738	-1.921456
32	1	0	-3.958025	2.708150	-1.005063
33	1	0	-5.270807	1.567226	-0.596676

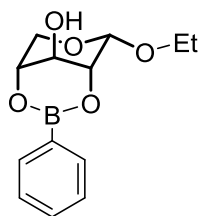


Ethyl α -D-xylofuranoside (mono-boronate 1,3 diol)

Energy: -867.416105211

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.295636	-0.037544	0.539105
2	8	0	2.809743	1.245421	0.188989
3	6	0	1.491704	1.146025	-0.396508
4	6	0	1.102167	-0.345938	-0.333773
5	6	0	2.047952	-0.914009	0.742326
6	8	0	4.042301	-0.636162	-0.497718
7	6	0	-2.724227	0.057123	-0.059089
8	6	0	-3.146022	-1.279019	-0.196931
9	6	0	0.532365	2.014211	0.419917
10	8	0	-0.270786	-0.586526	-0.048921
11	8	0	2.293908	-2.297038	0.667181
12	8	0	-0.825973	1.739113	0.075954
13	5	0	-1.206787	0.420486	-0.012994
14	6	0	-4.502954	-1.606274	-0.231803
15	6	0	-5.466891	-0.597923	-0.132288
16	6	0	-5.068893	0.735895	0.003626
17	6	0	-3.710597	1.056773	0.041602
18	6	0	5.304999	-0.020874	-0.753439
19	1	0	3.924261	0.089823	1.429034
20	1	0	1.539505	1.507857	-1.429079
21	1	0	1.322039	-0.841997	-1.285271
22	1	0	1.618691	-0.719981	1.730638
23	1	0	-2.398803	-2.063814	-0.273597
24	1	0	0.715118	3.075451	0.235057
25	1	0	0.688810	1.822569	1.489136
26	1	0	2.958904	-2.432306	-0.025976
27	1	0	-4.809770	-2.643391	-0.336329
28	1	0	-6.523548	-0.850390	-0.159935
29	1	0	-5.815999	1.521086	0.081644
30	1	0	-3.403873	2.093225	0.150703
31	1	0	5.932193	-0.034242	0.148463
32	1	0	5.175515	1.012377	-1.092342
33	1	0	5.785920	-0.607833	-1.537540

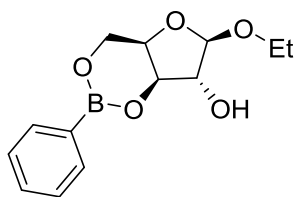


Ethyl α -D-xylopyranoside (mono-boronate 1,3 diol)

Energy: -867.414020429

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.804082	0.381474	1.276287
2	6	0	1.969997	-1.018943	1.502546
3	6	0	1.253742	-1.831930	0.419337
4	6	0	1.787190	-1.455227	-0.969954
5	6	0	1.545683	0.059604	-1.121299
6	6	0	2.288137	0.805164	0.002109
7	6	0	-2.168518	-0.127793	-0.108755
8	6	0	-3.033042	-0.923779	0.665980
9	8	0	-0.148067	-1.555960	0.456442
10	8	0	3.166150	-1.810042	-1.031363
11	8	0	0.144324	0.299917	-1.052626
12	8	0	2.071491	2.165894	-0.138652
13	6	0	2.824172	2.979483	0.760969
14	6	0	-4.393871	-0.626552	0.764422
15	5	0	-0.647487	-0.464102	-0.223302
16	6	0	-4.917293	0.478967	0.086404
17	6	0	-4.074985	1.283740	-0.687254
18	6	0	-2.715154	0.981007	-0.782079
19	1	0	3.034988	-1.290691	1.522716
20	1	0	1.526229	-1.221098	2.479619
21	1	0	1.390142	-2.901777	0.605908
22	1	0	1.210558	-1.992292	-1.734448
23	1	0	1.898332	0.434895	-2.088359
24	1	0	3.366292	0.568795	-0.061616
25	1	0	-2.629365	-1.782543	1.194966
26	1	0	3.462113	-1.785673	-1.950374
27	1	0	3.900971	2.778454	0.661655
28	1	0	2.516360	2.812021	1.797589
29	1	0	2.622345	4.014124	0.478873
30	1	0	-5.045428	-1.253103	1.367611
31	1	0	-5.975974	0.712759	0.161606
32	1	0	-4.478273	2.144772	-1.213444
33	1	0	-2.062044	1.609170	-1.381038

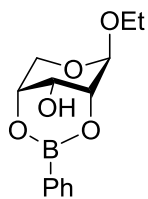


Ethyl β -D-xylofuranoside (mono-boronate 1,3-diol)

Energy: -867.413656399

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.266614	-0.361498	-0.016754
2	8	0	2.927929	0.564007	-1.059941
3	6	0	1.506774	0.634855	-1.208395
4	6	0	1.025058	-0.776275	-0.840707
5	6	0	2.012953	-1.208554	0.257893
6	8	0	3.632734	0.292728	1.168243
7	6	0	-2.639062	0.120346	-0.003965
8	6	0	-3.254478	-1.145489	-0.030466
9	6	0	0.870215	1.688545	-0.295513
10	8	0	-0.336638	-0.852551	-0.428221
11	8	0	2.362432	-2.584722	0.219490
12	8	0	-0.554419	1.536235	-0.278279
13	5	0	-1.104136	0.279353	-0.249136
14	6	0	-4.625239	-1.286824	0.194685
15	6	0	-5.409952	-0.158067	0.451218
16	6	0	-4.818744	1.108952	0.481027
17	6	0	-3.447272	1.243329	0.256509
18	6	0	4.876323	0.988919	1.086765
19	1	0	4.100076	-0.969069	-0.391307
20	1	0	1.302017	0.879379	-2.255112
21	1	0	1.145301	-1.450675	-1.695570
22	1	0	1.614749	-0.936059	1.242828
23	1	0	-2.648200	-2.024390	-0.231006
24	1	0	1.089858	2.697005	-0.654620
25	1	0	1.260589	1.595167	0.724112
26	1	0	1.611142	-3.104122	0.535049
27	1	0	-5.082062	-2.272444	0.170090
28	1	0	-6.477007	-0.265362	0.626699
29	1	0	-5.426046	1.987734	0.680074
30	1	0	-2.990127	2.228392	0.281881
31	1	0	4.827769	1.801627	0.353765
32	1	0	5.689519	0.301359	0.815202
33	1	0	5.067674	1.399676	2.079470

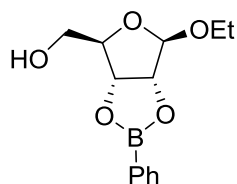


Ethyl- β -D-ribofuranoside (mono-boronate 1,3-diol)

Energy: -867.421441473

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.774384	0.731982	1.251291
2	6	0	1.917451	-0.643048	1.627580
3	6	0	1.194513	-1.570619	0.646150
4	6	0	1.749024	-1.349006	-0.765998
5	6	0	1.466054	0.120681	-1.096066
6	6	0	2.174292	1.033566	-0.074809
7	5	0	-0.724917	-0.280259	-0.113568
8	6	0	-2.243618	0.070383	-0.017685
9	8	0	-0.214675	-1.293982	0.666330
10	8	0	1.219995	-2.248850	-1.727015
11	8	0	0.059267	0.379719	-1.036546
12	8	0	3.556215	0.879757	-0.279836
13	6	0	4.361817	1.834400	0.412462
14	6	0	-3.086232	-0.598938	0.889992
15	6	0	-4.444544	-0.287646	0.976906
16	6	0	-4.987348	0.703367	0.152859
17	6	0	-4.167672	1.380102	-0.755925
18	6	0	-2.809957	1.064946	-0.837501
19	1	0	2.978576	-0.922161	1.681804
20	1	0	1.474933	-0.720664	2.622737
21	1	0	1.319654	-2.613079	0.955542
22	1	0	2.828817	-1.515332	-0.768928
23	1	0	1.802075	0.369712	-2.105188
24	1	0	1.867496	2.077319	-0.219582
25	1	0	0.259212	-2.144947	-1.772060
26	1	0	4.239336	1.747271	1.497563
27	1	0	4.106049	2.856521	0.101345
28	1	0	5.396912	1.621859	0.140128
29	1	0	-2.666904	-1.369153	1.531088
30	1	0	-5.079357	-0.814422	1.684141
31	1	0	-6.044286	0.947306	0.218641
32	1	0	-4.587033	2.150469	-1.397298
33	1	0	-2.175056	1.592466	-1.543676

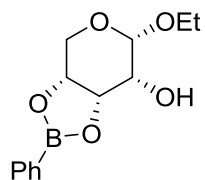


Ethyl- β -D-ribofuranoside (mono-boronate)

Energy: -867.420218811

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.026090	-0.986087	-0.619283
2	6	0	1.867170	-1.417818	0.592356
3	8	0	1.995678	-0.223547	1.405180
4	6	0	1.952217	0.924332	0.612569
5	6	0	1.105524	0.567026	-0.630237
6	6	0	3.230208	-2.008555	0.225656
7	8	0	3.934074	-1.267608	-0.759382
8	8	0	-0.369364	-1.275448	-0.425059
9	8	0	3.290332	1.280442	0.254843
10	8	0	-0.247127	1.014922	-0.481235
11	5	0	-1.065388	-0.090353	-0.347098
12	6	0	3.458594	2.643767	-0.125403
13	6	0	-2.600122	-0.002376	-0.139597
14	6	0	-3.250696	1.244044	-0.067443
15	6	0	-4.632149	1.323737	0.117060
16	6	0	-5.388907	0.153390	0.233045
17	6	0	-4.761035	-1.094348	0.163776
18	6	0	-3.379411	-1.168911	-0.021107
19	1	0	1.359967	-1.456833	-1.545452
20	1	0	1.315179	-2.140856	1.200872
21	1	0	1.505775	1.737720	1.197201
22	1	0	1.527910	0.990020	-1.544310
23	1	0	3.071969	-3.007387	-0.196386
24	1	0	3.820719	-2.118351	1.146381
25	1	0	4.061593	-0.361066	-0.427605
26	1	0	3.134730	3.314513	0.681749
27	1	0	2.901611	2.887769	-1.039998
28	1	0	4.524461	2.788322	-0.308450
29	1	0	-2.665659	2.155190	-0.157256
30	1	0	-5.118895	2.293580	0.170557
31	1	0	-6.464320	0.213546	0.376657
32	1	0	-5.347729	-2.004309	0.253612
33	1	0	-2.894013	-2.139405	-0.075214

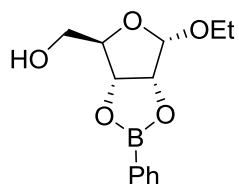


Ethyl- α -D-ribofuranoside (mono-boronate)

Energy: -867.416638695

Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.024271	1.727919	-0.529937
2	6	0	-1.733892	1.621843	0.829984
3	8	0	-3.052310	1.080850	0.702111
4	6	0	-3.062072	-0.257717	0.217017
5	6	0	-2.512466	-0.295093	-1.218405
6	6	0	-1.183196	0.453692	-1.388212
7	8	0	0.399400	1.796370	-0.303554
8	8	0	-2.313791	-1.135938	1.013299
9	5	0	0.897094	0.516832	-0.480224
10	6	0	-2.906045	-1.438537	2.276159
11	8	0	-2.445553	-1.607564	-1.735257
12	8	0	-0.045860	-0.348016	-0.998268
13	6	0	2.353030	0.105886	-0.137368
14	6	0	2.813505	-1.200289	-0.390867
15	6	0	4.123706	-1.572342	-0.084720
16	6	0	4.999579	-0.639585	0.479818
17	6	0	4.561755	0.663450	0.737570
18	6	0	3.249955	1.030121	0.431588
19	1	0	-1.340578	2.624773	-1.068789
20	1	0	-1.855330	2.607271	1.283879
21	1	0	-1.131109	0.998366	1.499716
22	1	0	-4.121419	-0.546047	0.219787
23	1	0	-3.251501	0.234138	-1.830148
24	1	0	-1.057981	0.686250	-2.453410
25	1	0	-3.899055	-1.888626	2.140858
26	1	0	-2.998914	-0.541531	2.899027
27	1	0	-2.246101	-2.157072	2.765094
28	1	0	-1.769120	-2.077840	-1.224439
29	1	0	2.136009	-1.926014	-0.832124
30	1	0	4.463255	-2.584482	-0.286395
31	1	0	6.020219	-0.927037	0.717520
32	1	0	5.241632	1.389044	1.175379
33	1	0	2.911922	2.042942	0.632753



Ethyl- α -D-ribofuranoside (mono-boronate)

Energy: -867.414944379

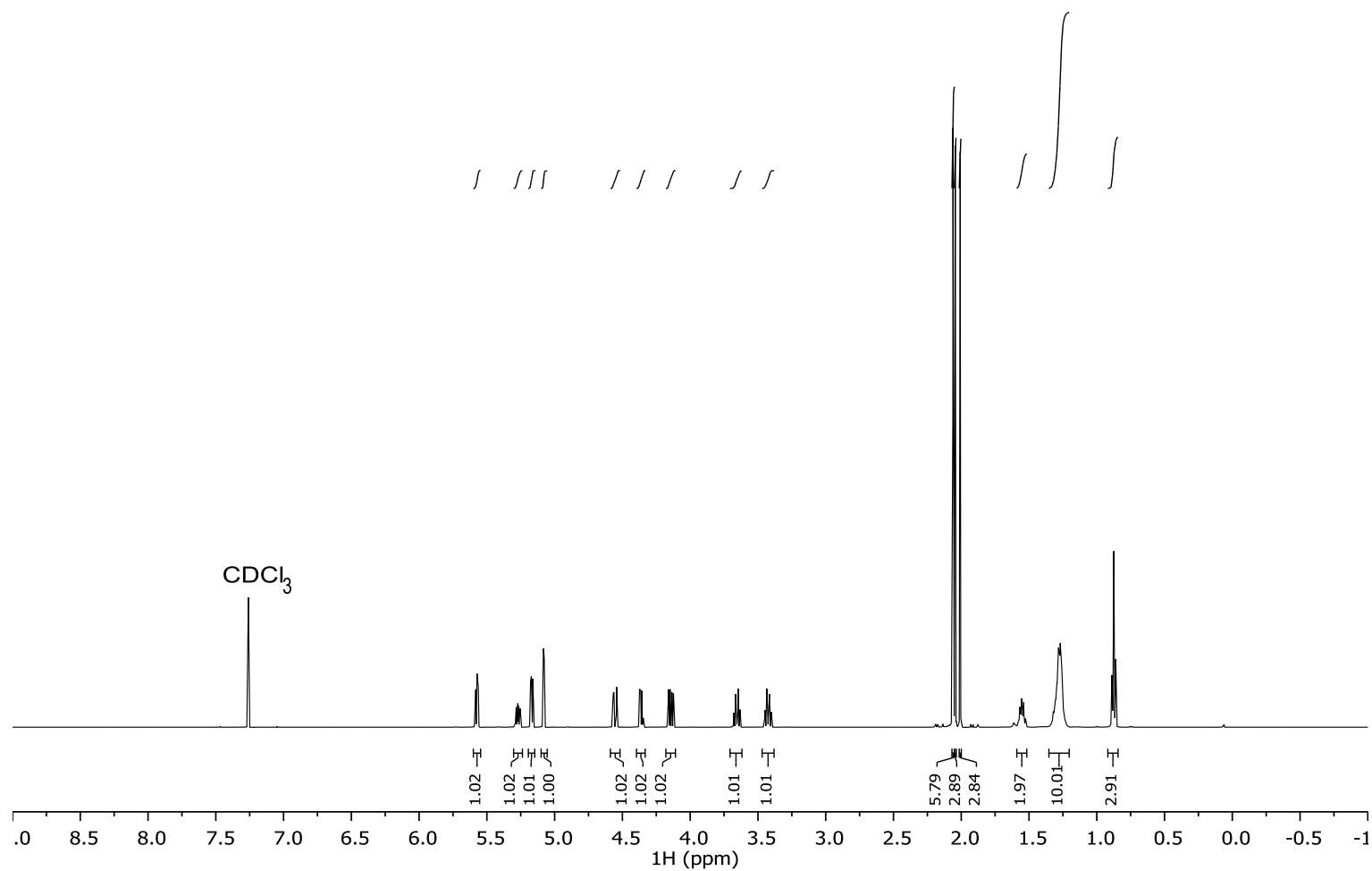
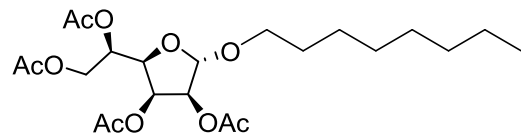
Imaginary Frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.442700	-0.897531	0.517340
2	6	0	-2.455158	-0.713330	-0.628456
3	8	0	-3.003225	0.612454	-0.423069
4	6	0	-1.997697	1.442044	0.101551
5	6	0	-1.255353	0.520383	1.115383
6	6	0	-3.625184	-1.686010	-0.633257
7	8	0	-4.356424	-1.656378	0.586790
8	8	0	-0.131997	-1.268285	0.060514
9	8	0	-1.157407	1.860309	-0.946634
10	8	0	0.153519	0.730462	1.163628
11	5	0	0.760363	-0.297861	0.464043
12	6	0	2.286568	-0.363295	0.190965
13	6	0	3.149185	0.647248	0.656105
14	6	0	4.522796	0.588713	0.413663
15	6	0	5.058962	-0.486084	-0.302590
16	6	0	4.218674	-1.500464	-0.772562
17	6	0	2.846104	-1.438145	-0.525550
18	6	0	-0.546991	3.134270	-0.756513
19	1	0	-1.786763	-1.638630	1.242690
20	1	0	-1.928527	-0.753276	-1.590265
21	1	0	-2.490476	2.305531	0.566089
22	1	0	-1.676071	0.633658	2.117810
23	1	0	-3.248445	-2.706810	-0.748685
24	1	0	-4.277587	-1.462854	-1.488727
25	1	0	-4.694560	-0.756399	0.696496
26	1	0	2.736175	1.482990	1.214297
27	1	0	5.174390	1.376732	0.780972
28	1	0	6.127722	-0.533475	-0.493078
29	1	0	4.633809	-2.336639	-1.328319
30	1	0	2.195905	-2.228265	-0.890651
31	1	0	0.148466	3.127832	0.090186
32	1	0	-1.309542	3.911468	-0.601528
33	1	0	0.002729	3.352154	-1.673806

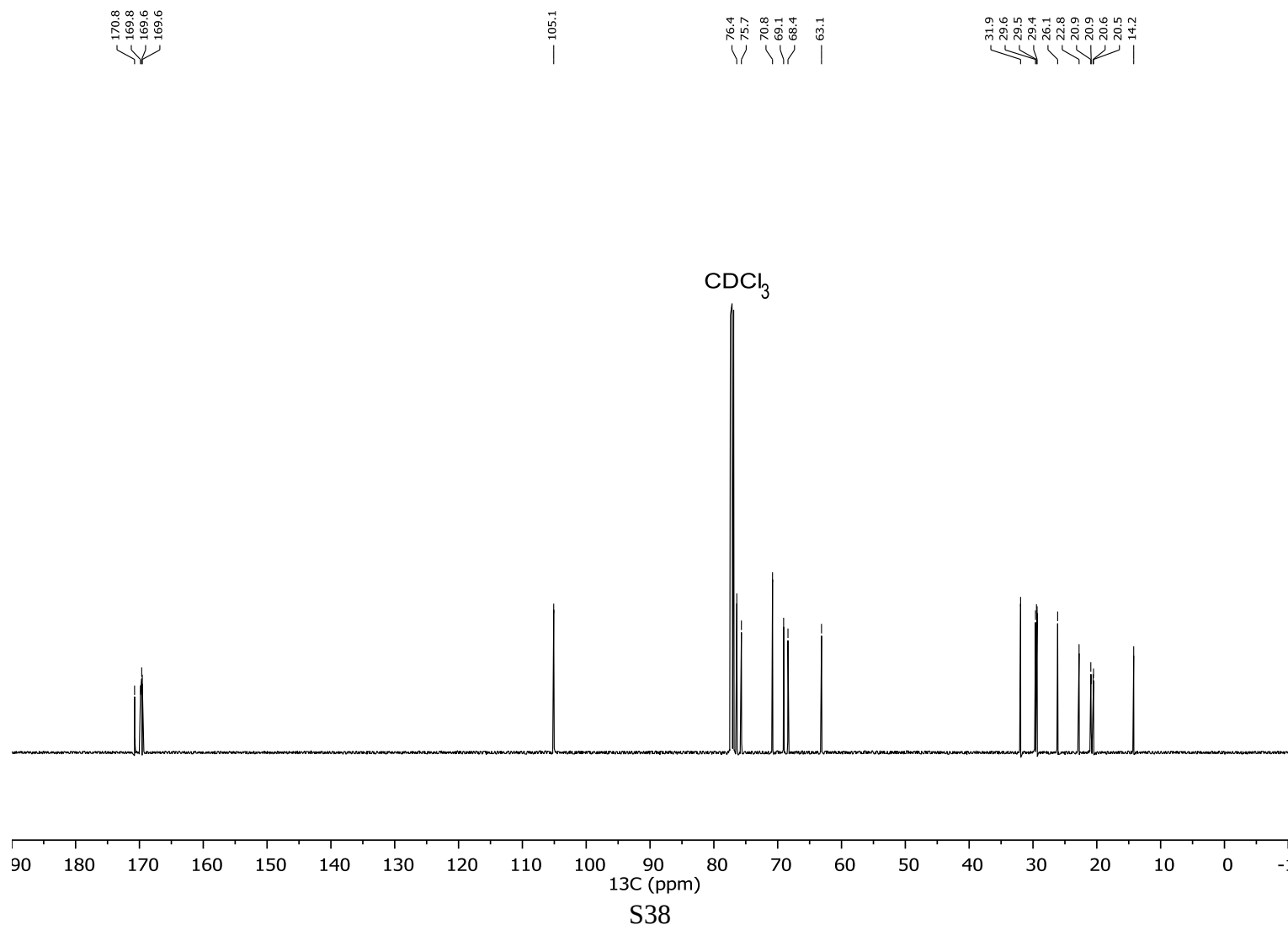
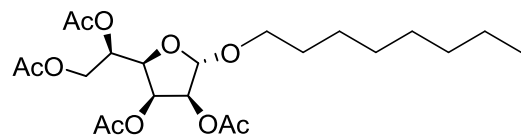
^1H , ^{13}C , and 2D NMR Spectra

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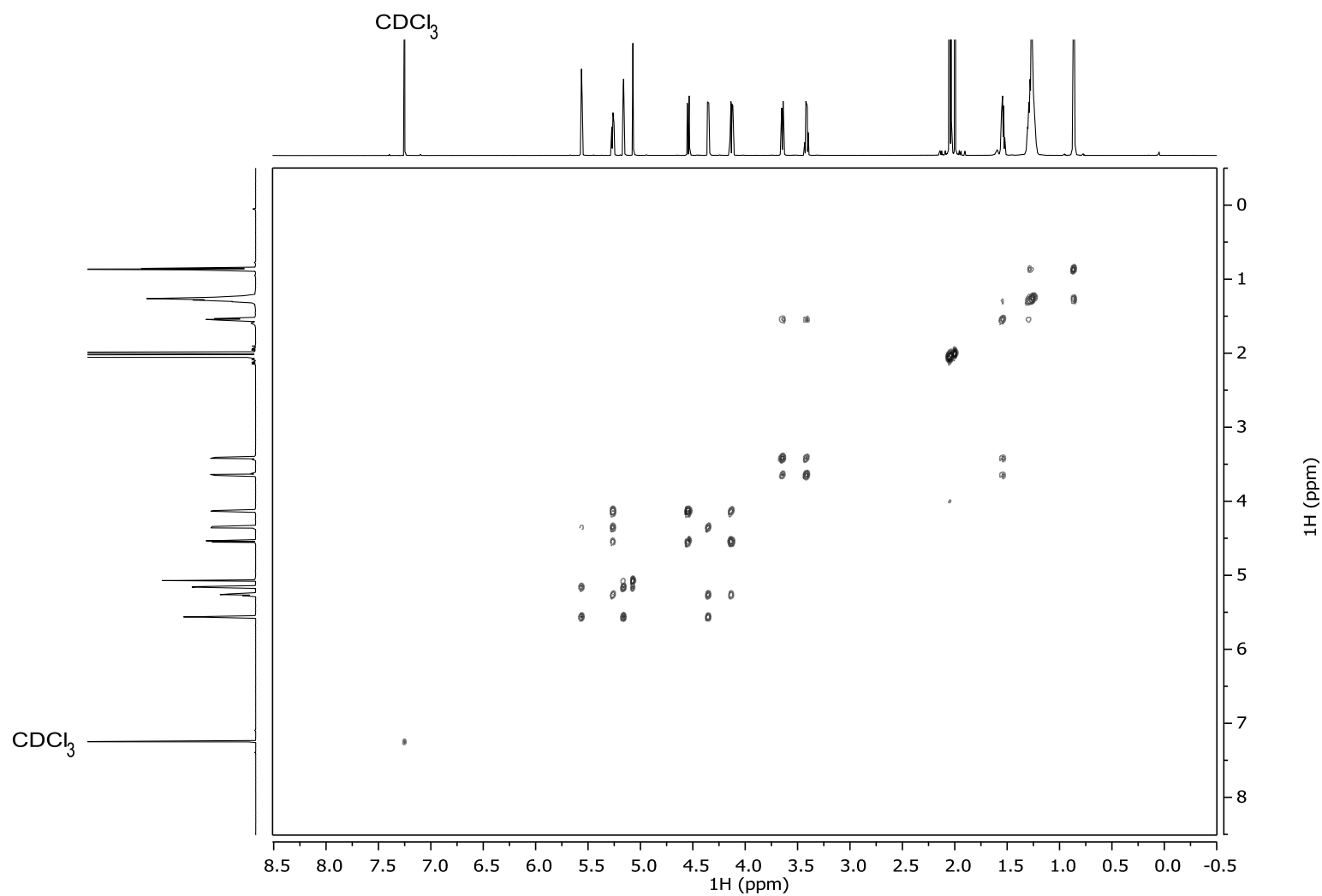
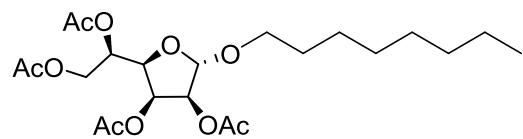
¹H NMR (500 MHz, CDCl₃) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- α -D-mannofuranoside



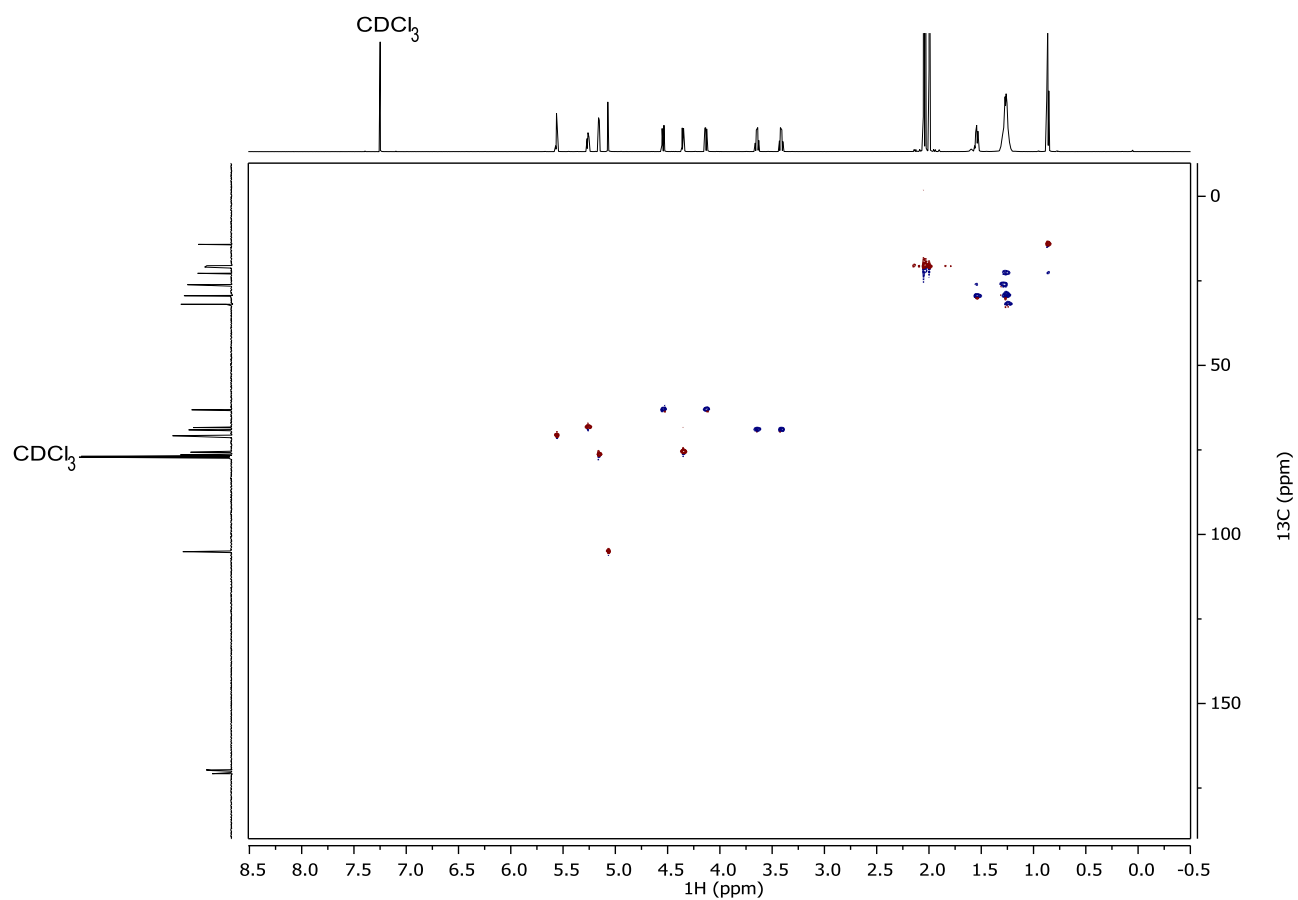
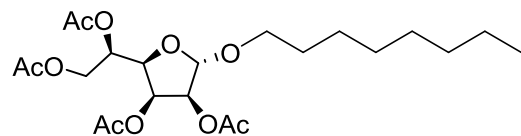
^{13}C NMR (125 MHz, CDCl_3) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- α -D-mannofuranoside



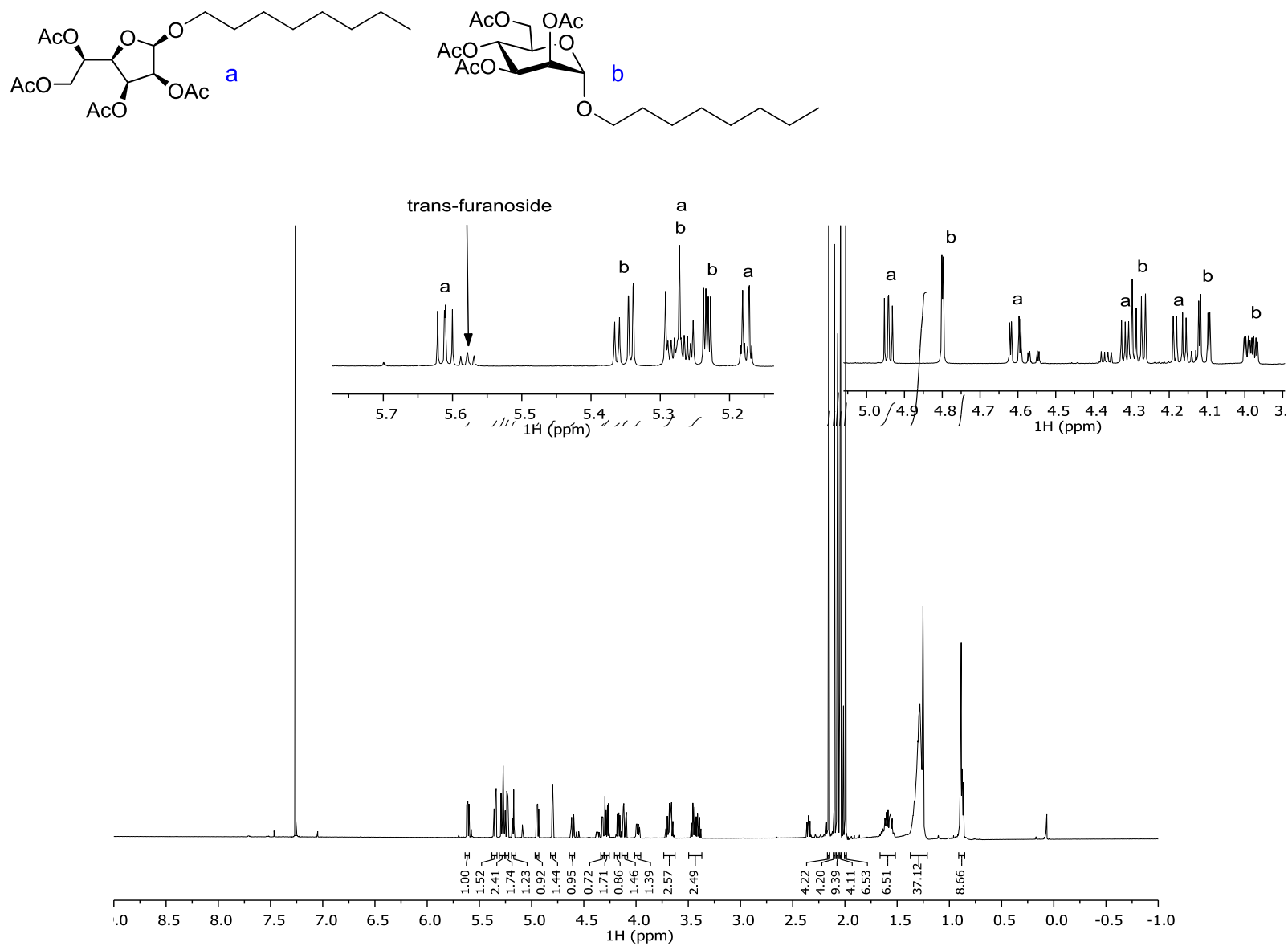
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- α -D-mannofuranoside



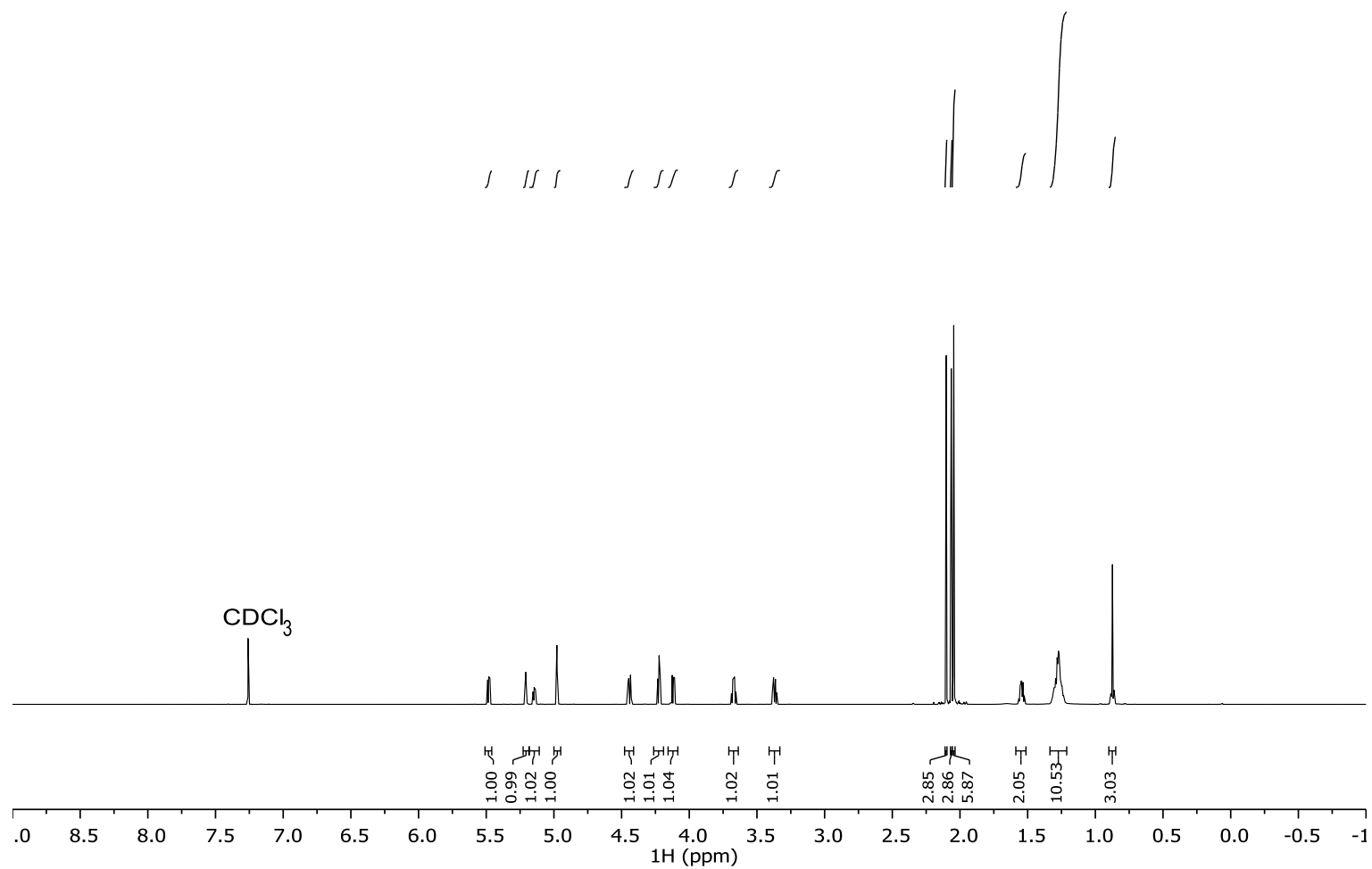
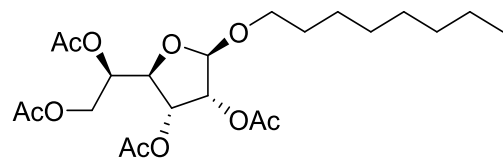
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- α -D-mannofuranoside



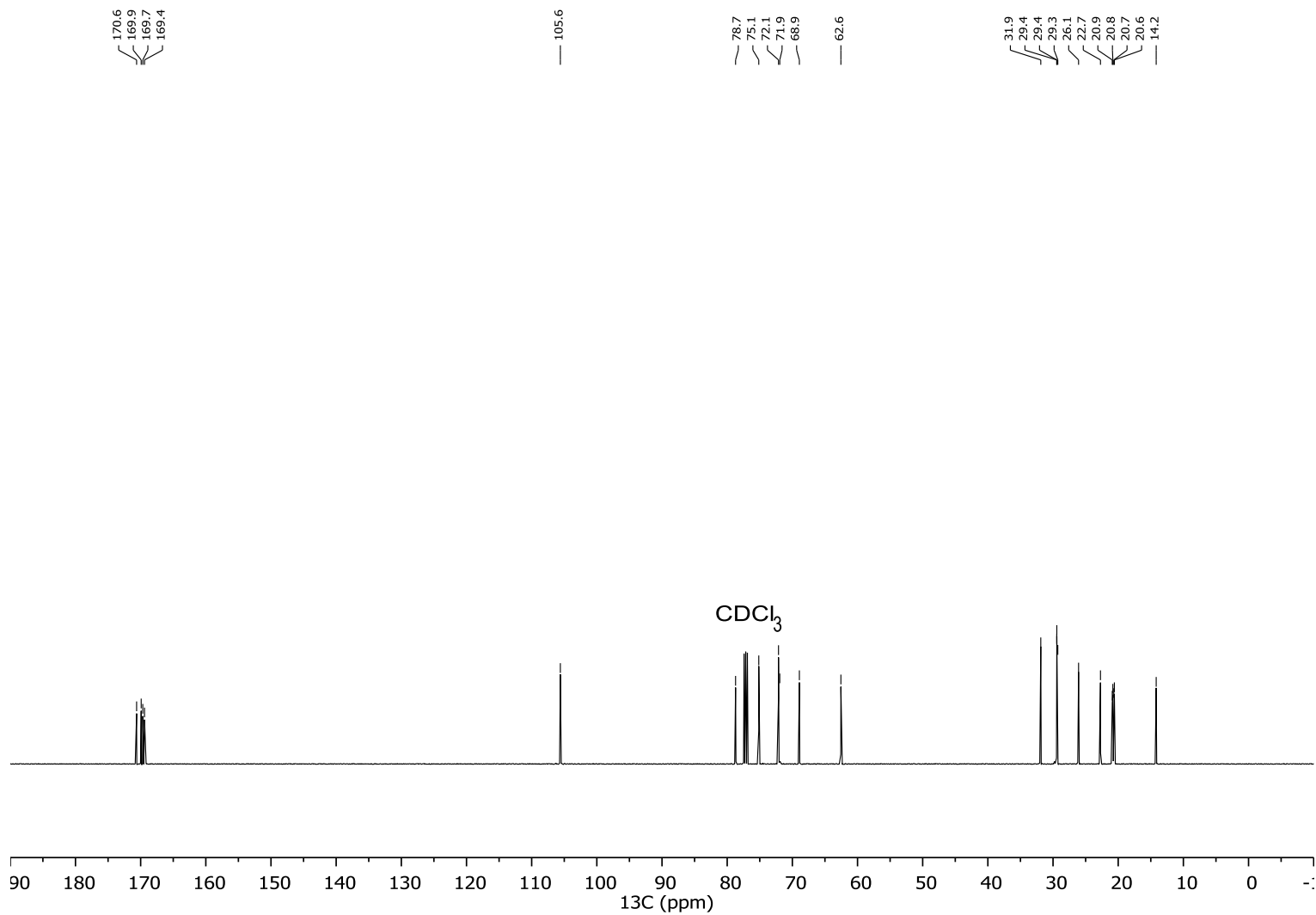
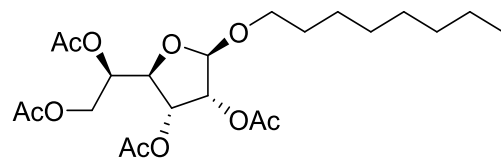
^1H NMR (500 MHz, CDCl_3) mixture of minor products **a** and **b**.
n-octyl 2,3,5,6-tetra-*O*-acetyl- β -D-mannofuranoside + *n*-octyl 2,3,5,6-tetra-*O*-acetyl- α -D-mannopyranoside



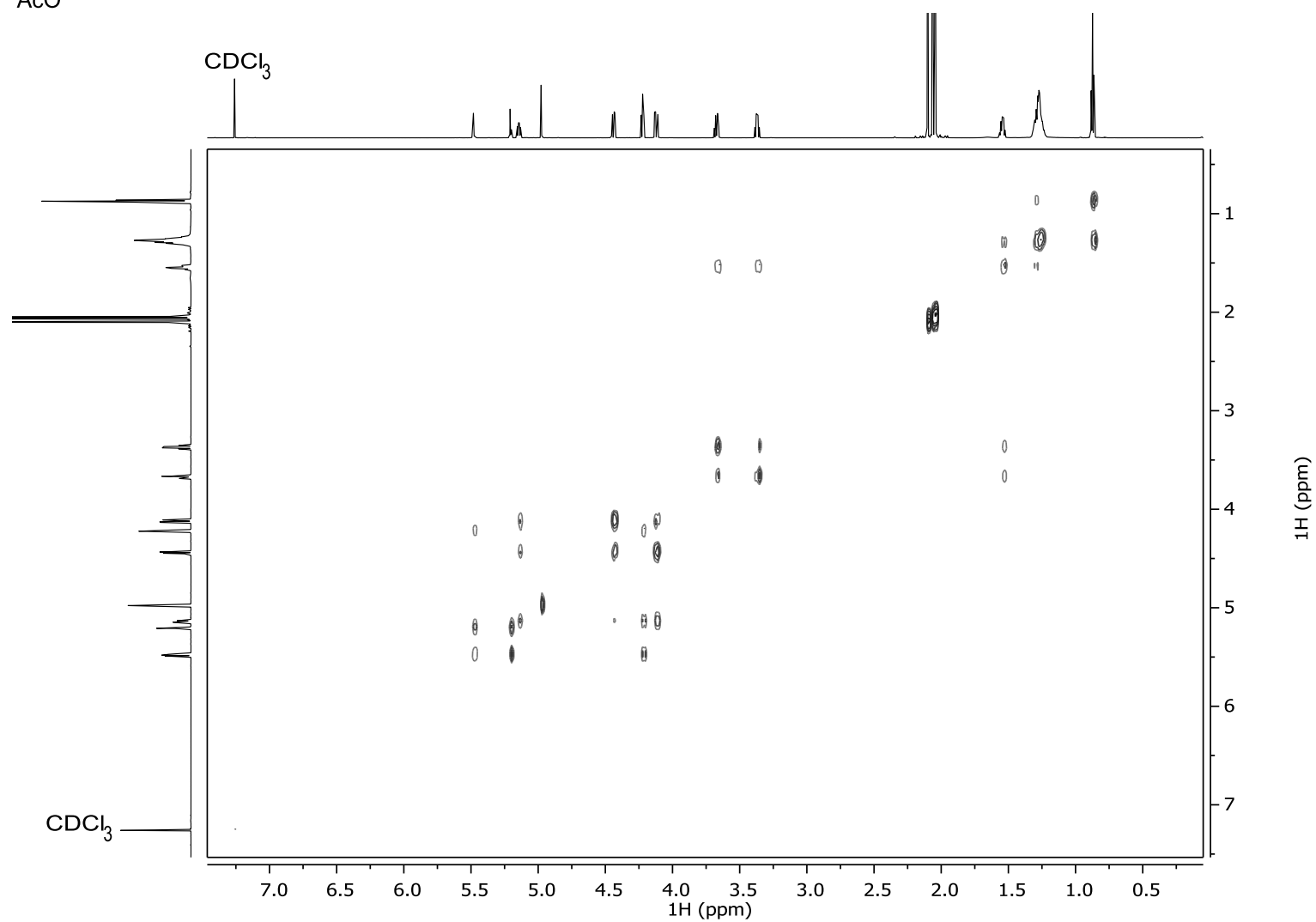
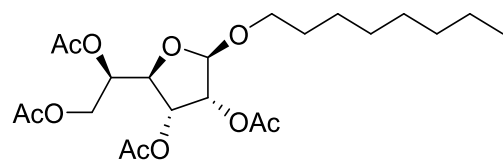
¹H NMR (700 MHz, CDCl₃) *n*-octyl-2,3,5,6-tetra-*O*-acetyl-β-D-allofuranoside



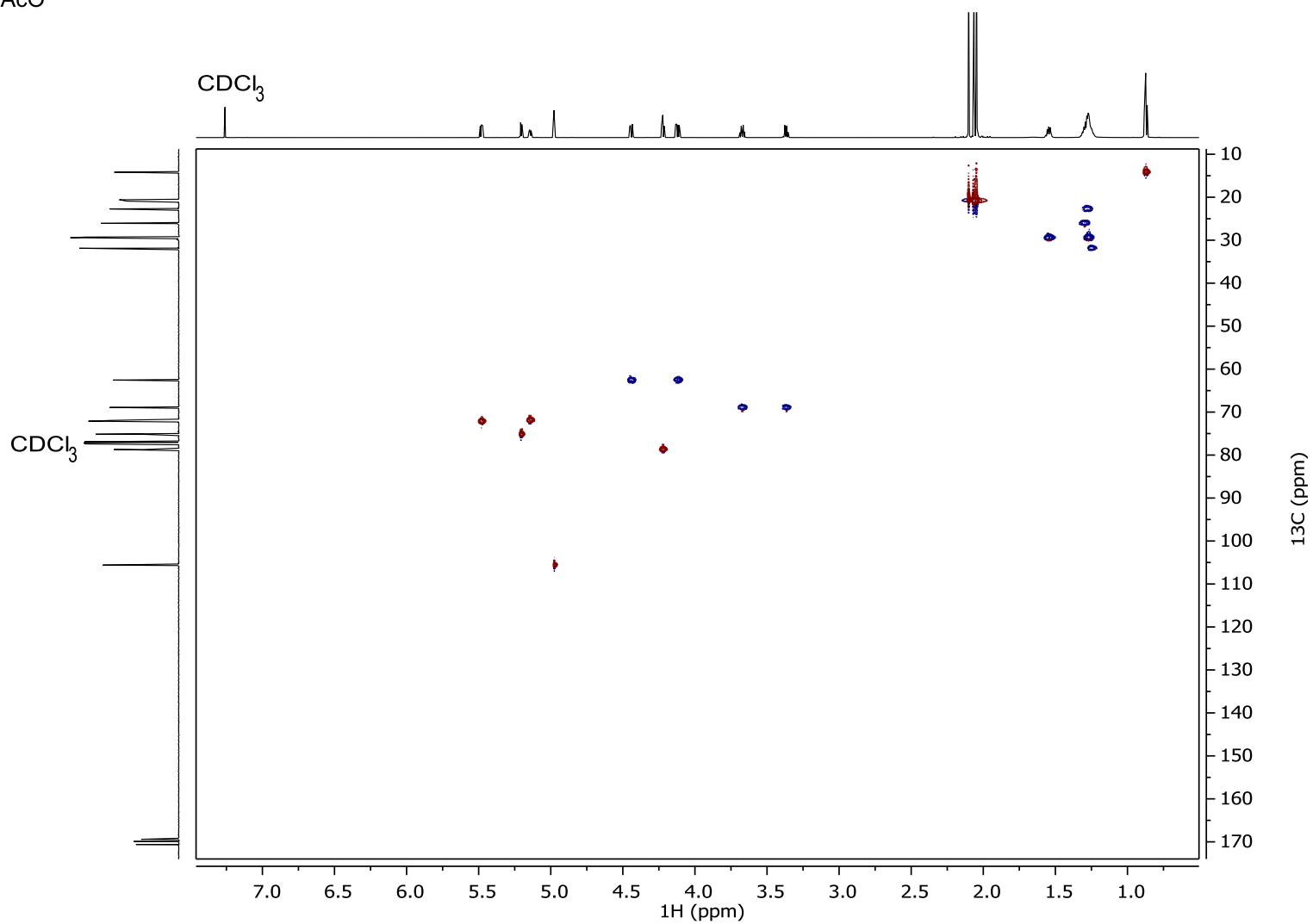
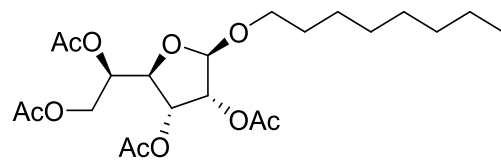
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- β -D-allofuranoside



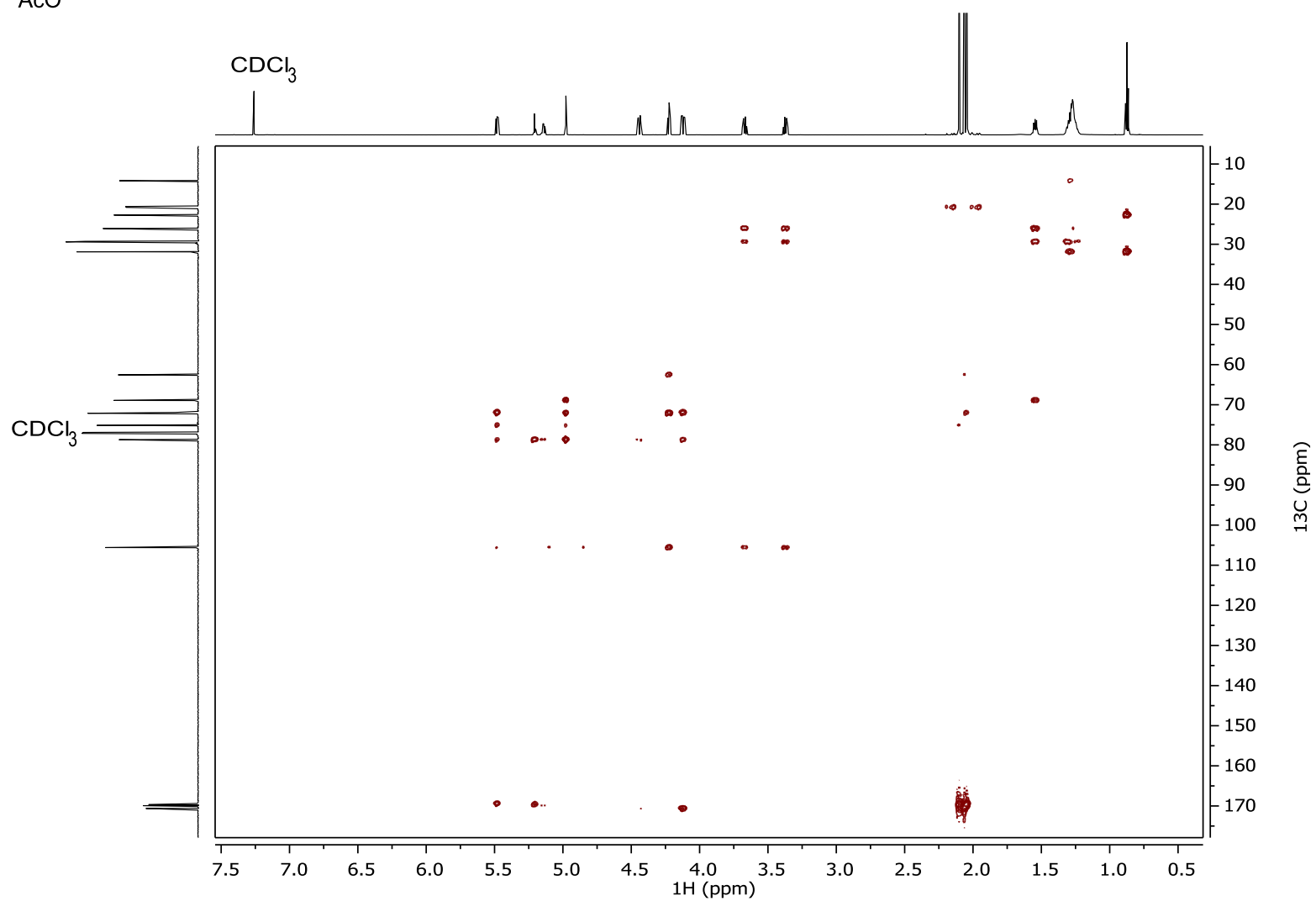
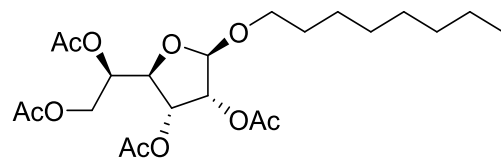
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- β -D-allofuranoside



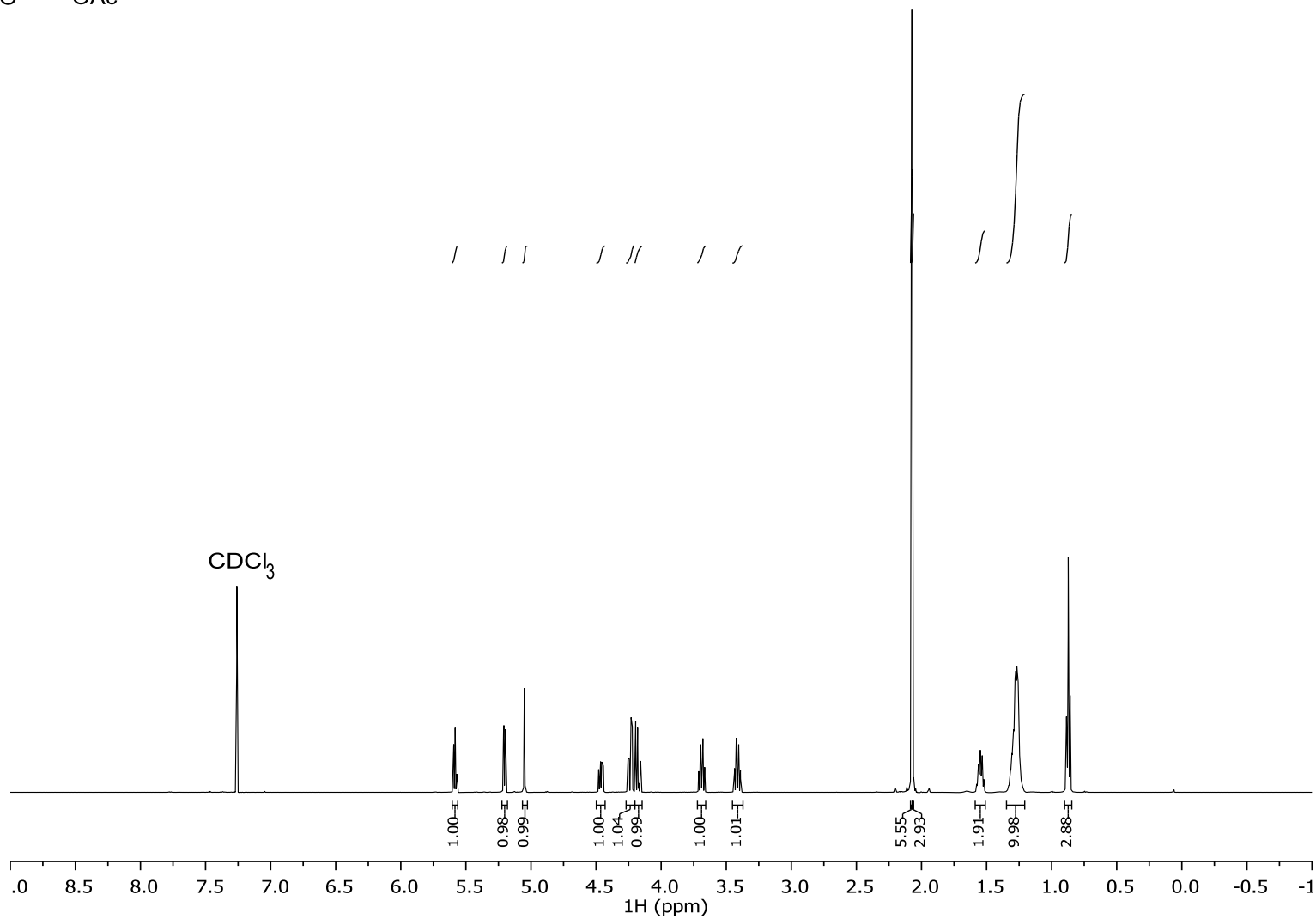
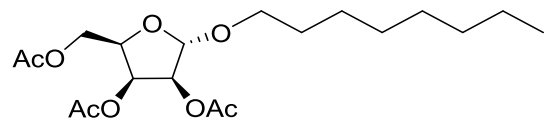
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- β -D-allofuranoside



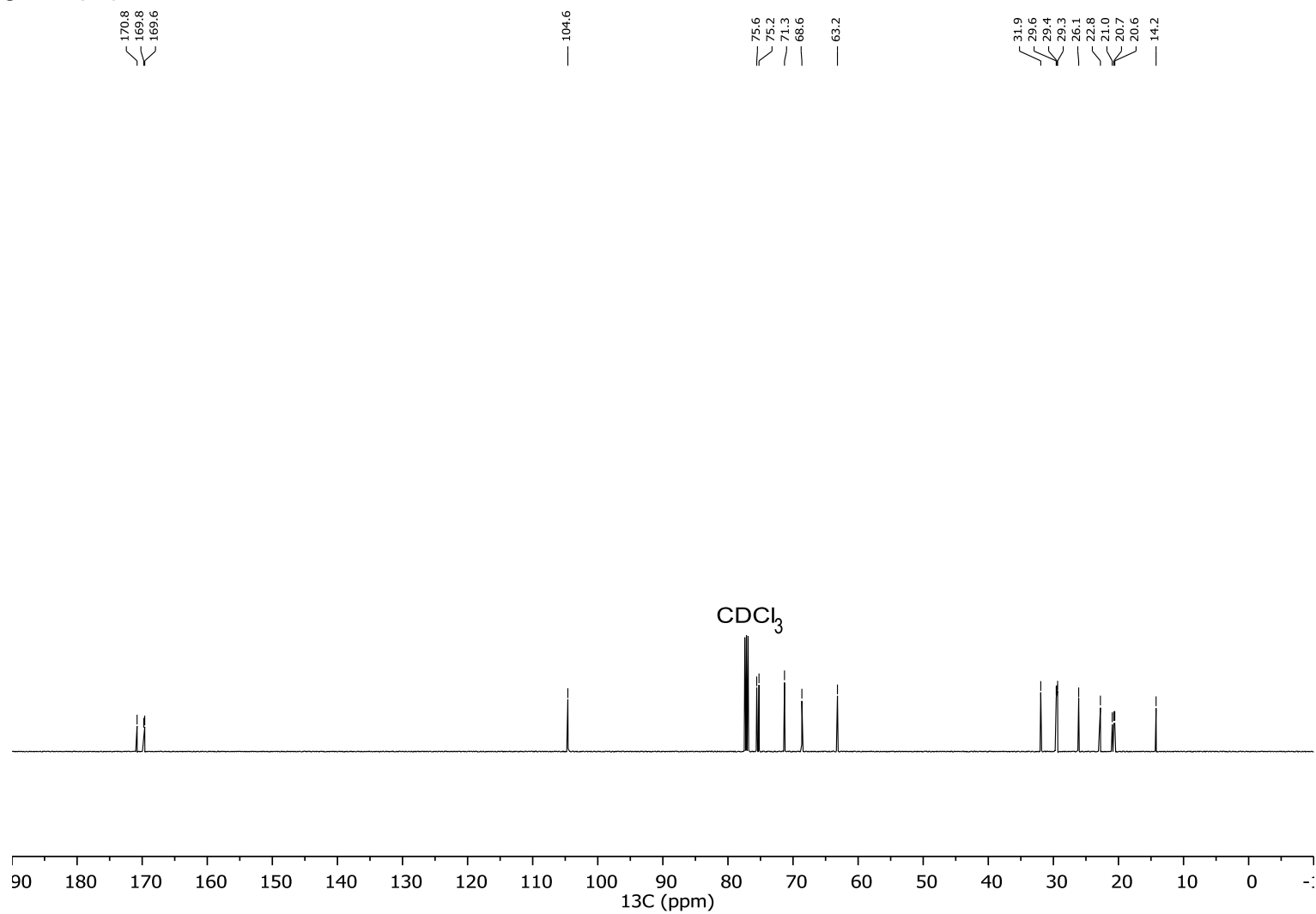
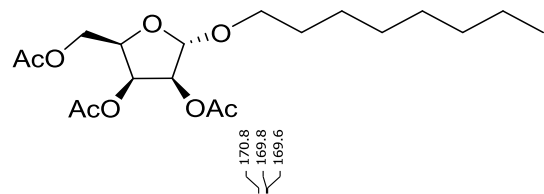
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl-2,3,5,6-tetra-*O*-acetyl- β -D-allofuranoside



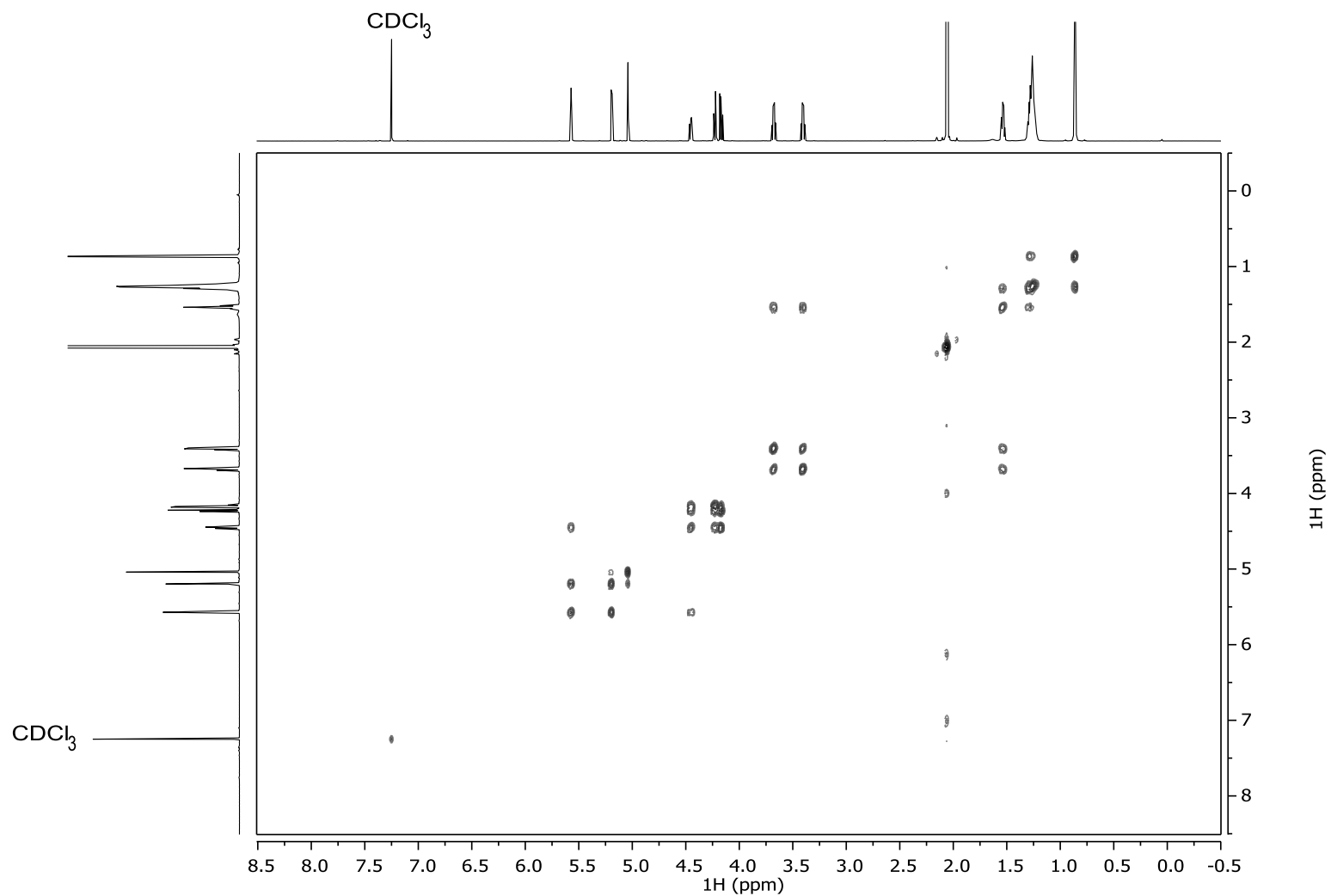
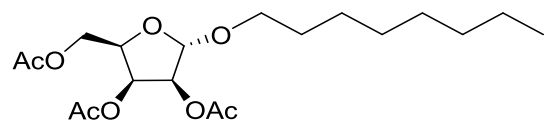
¹H NMR (500 MHz, CDCl₃) n-octyl 2,3,5-tri-*O*-acetyl- α -D-lyxofuranoside



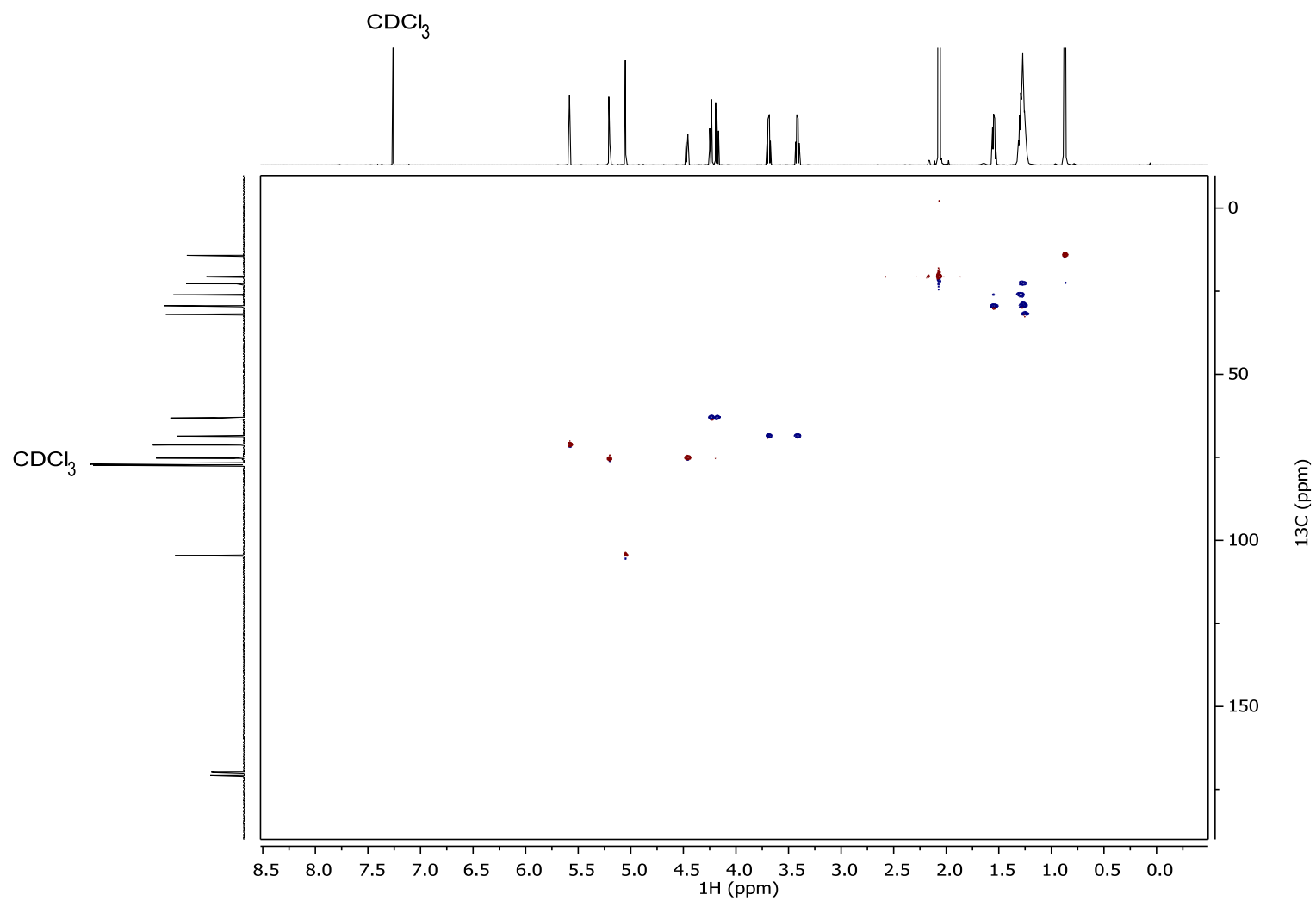
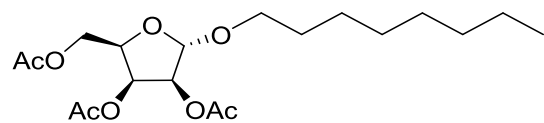
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-lyxofuranoside



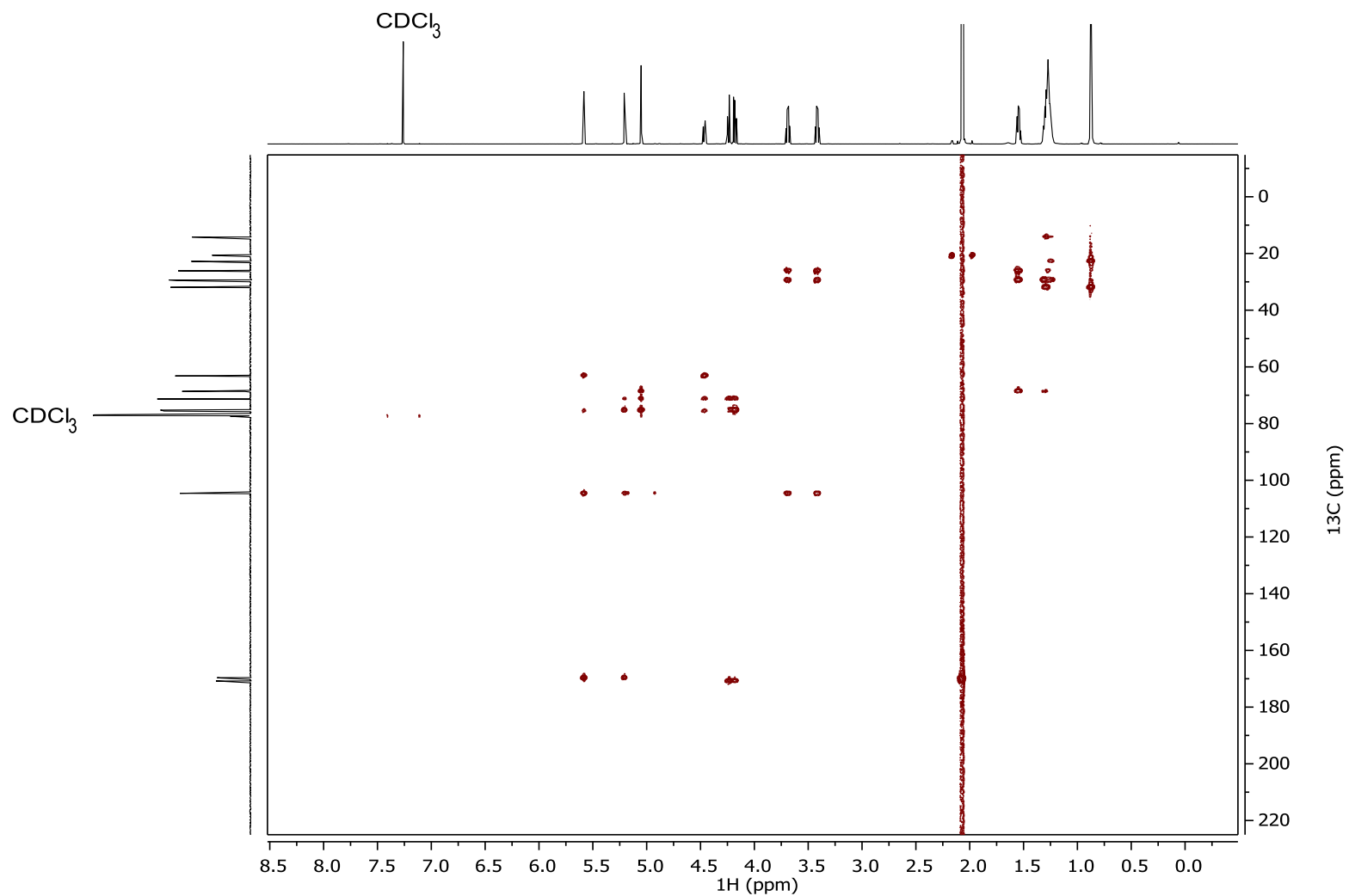
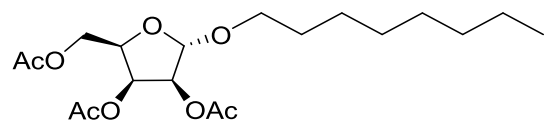
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-lyxofuranoside



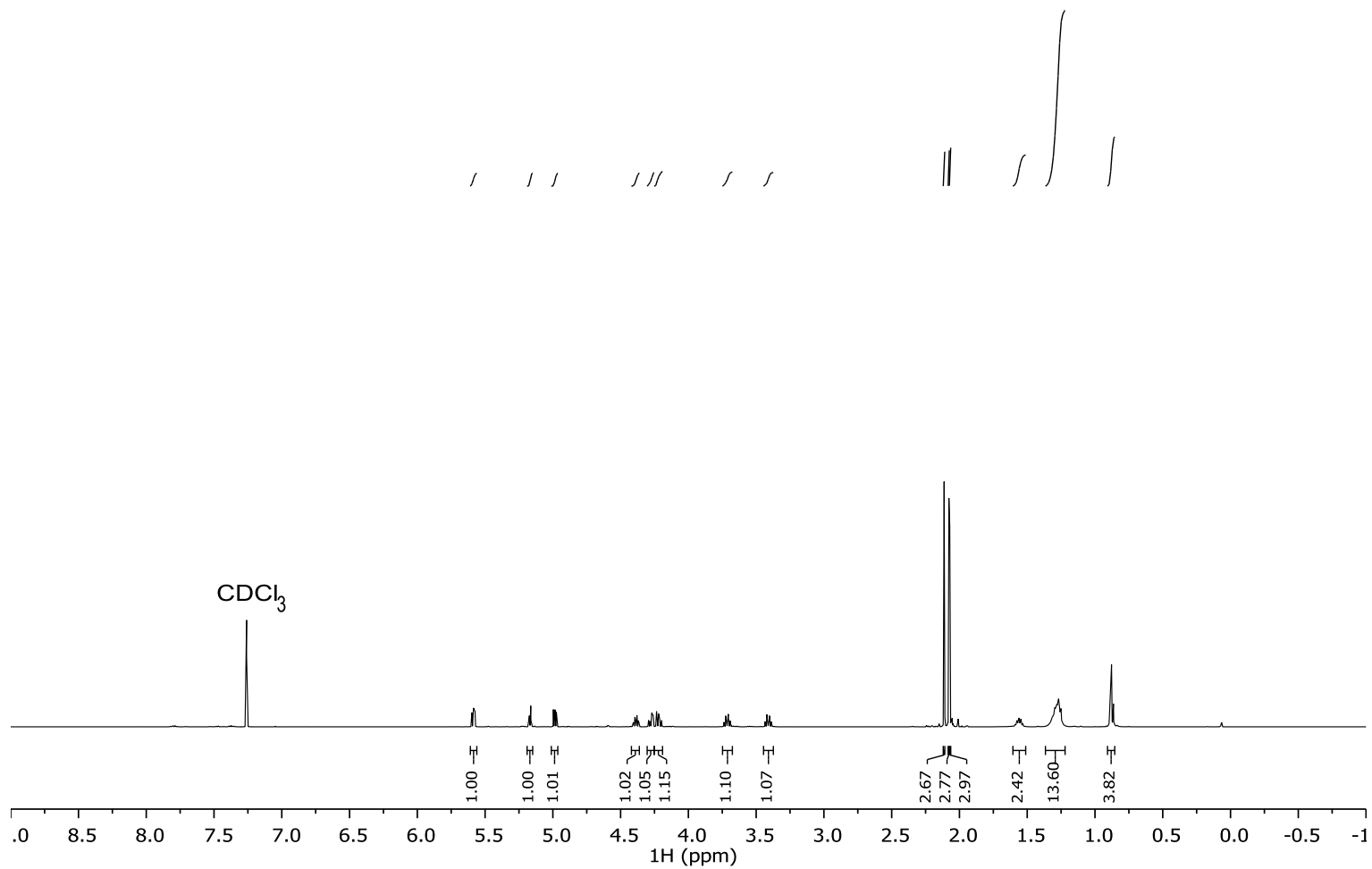
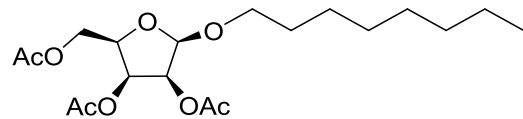
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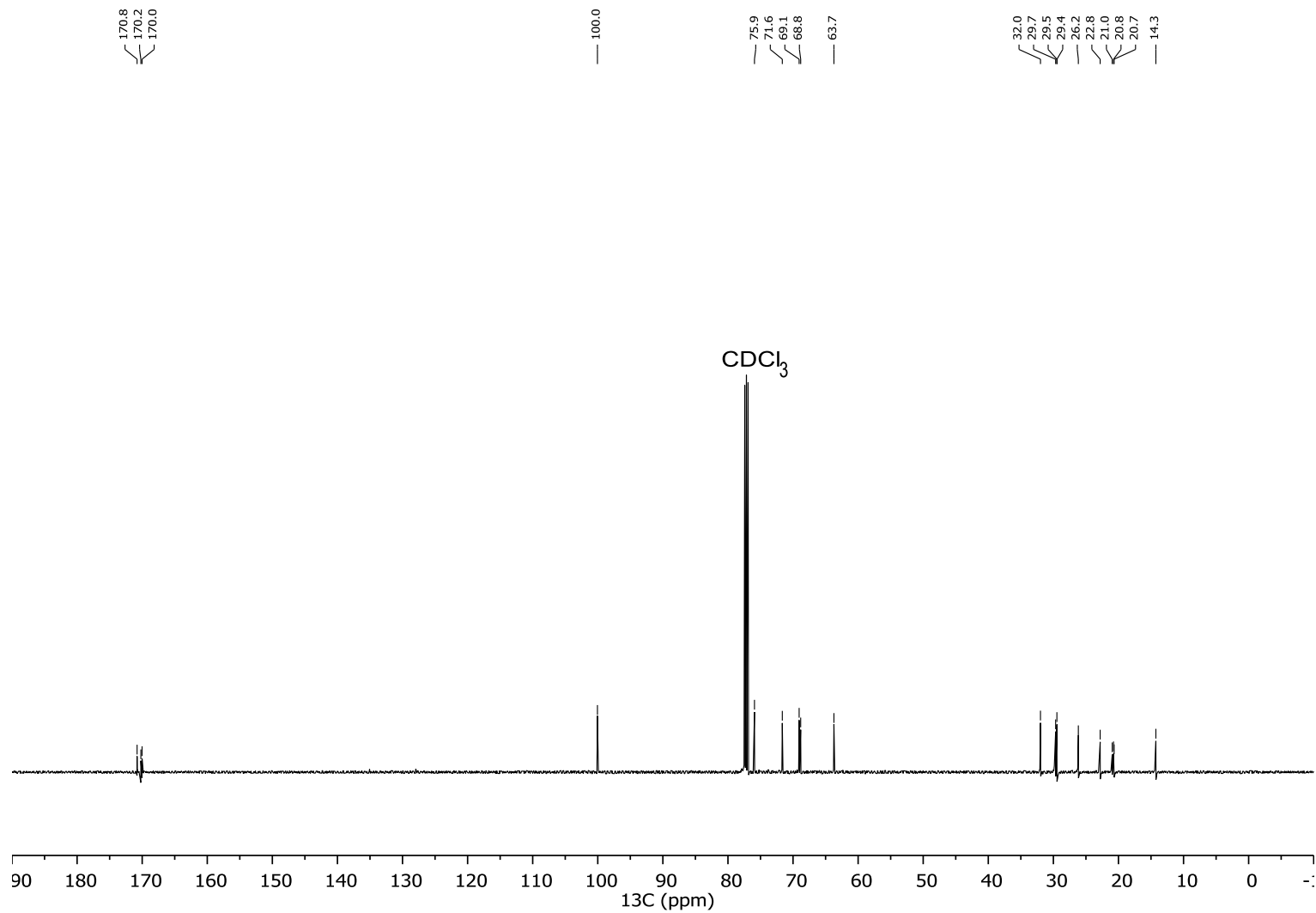
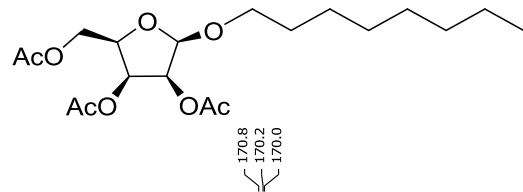
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-lyxofuranoside



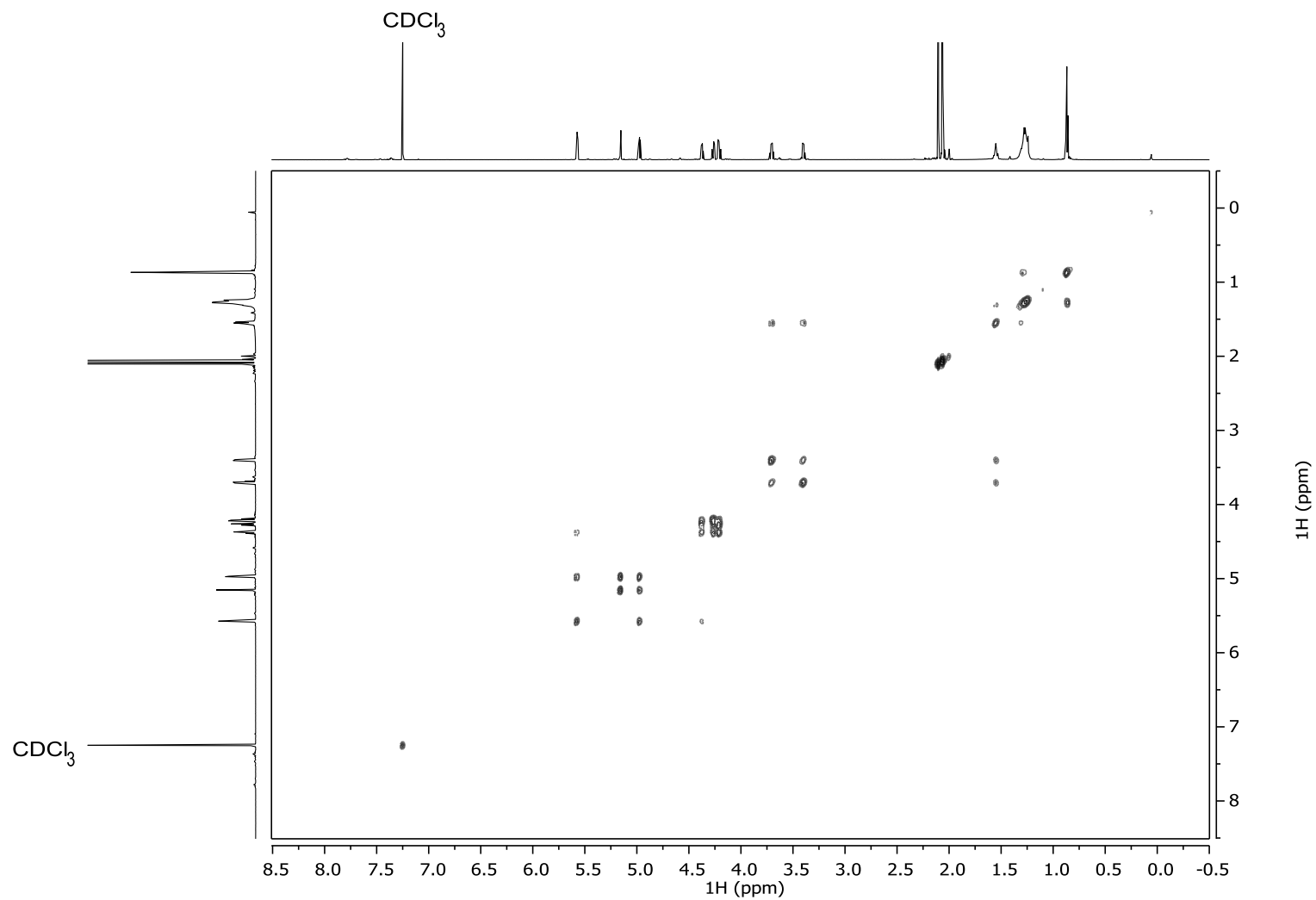
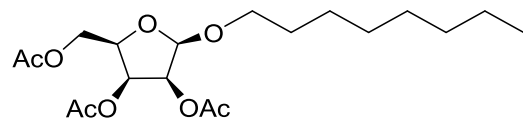
¹H NMR (500 MHz, CDCl₃) *n*-octyl 2,3,5-tri-*O*-acetyl-β-*D*-lyxofuranoside



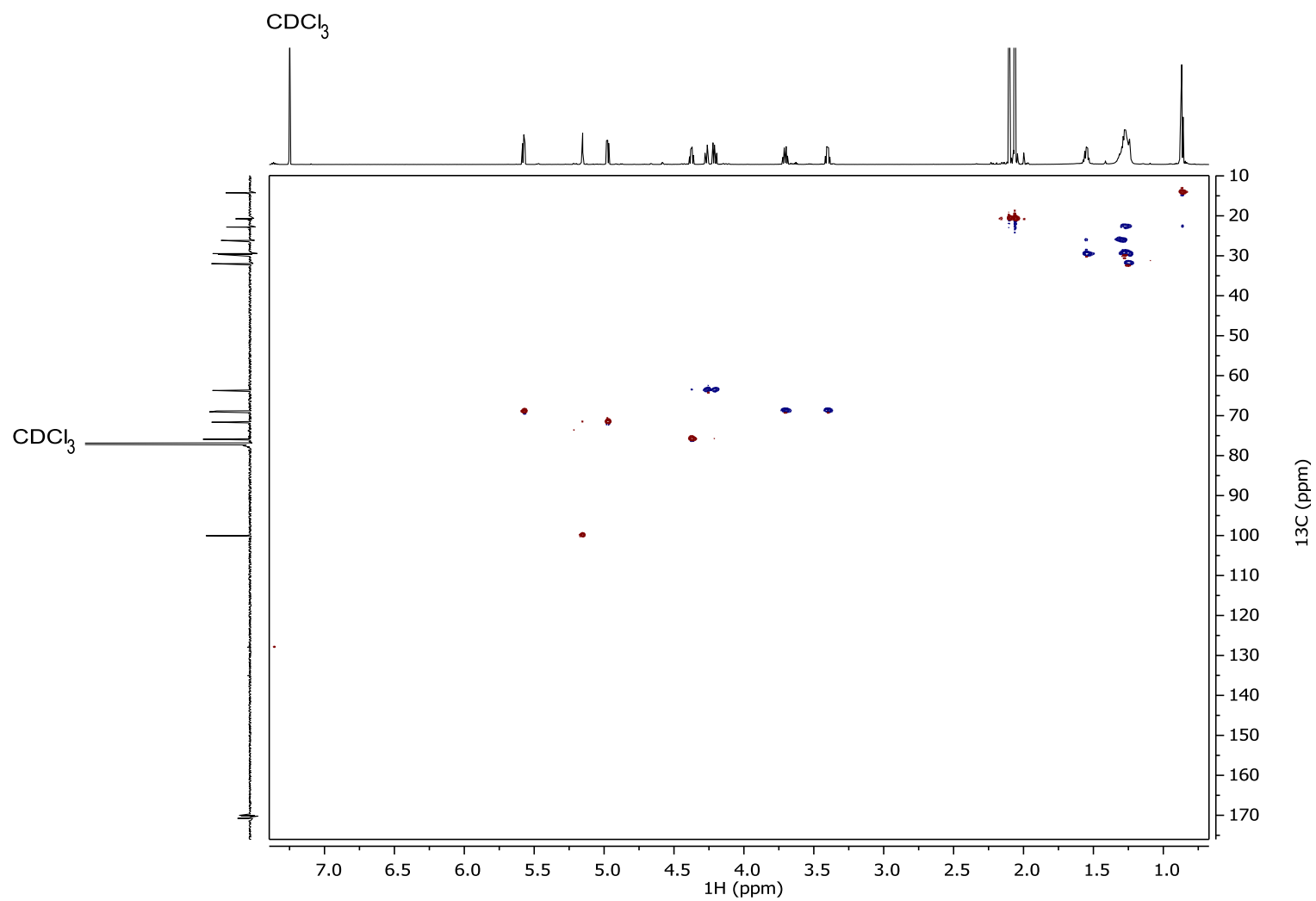
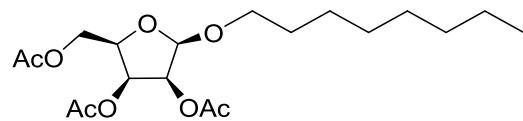
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-lyxofuranoside



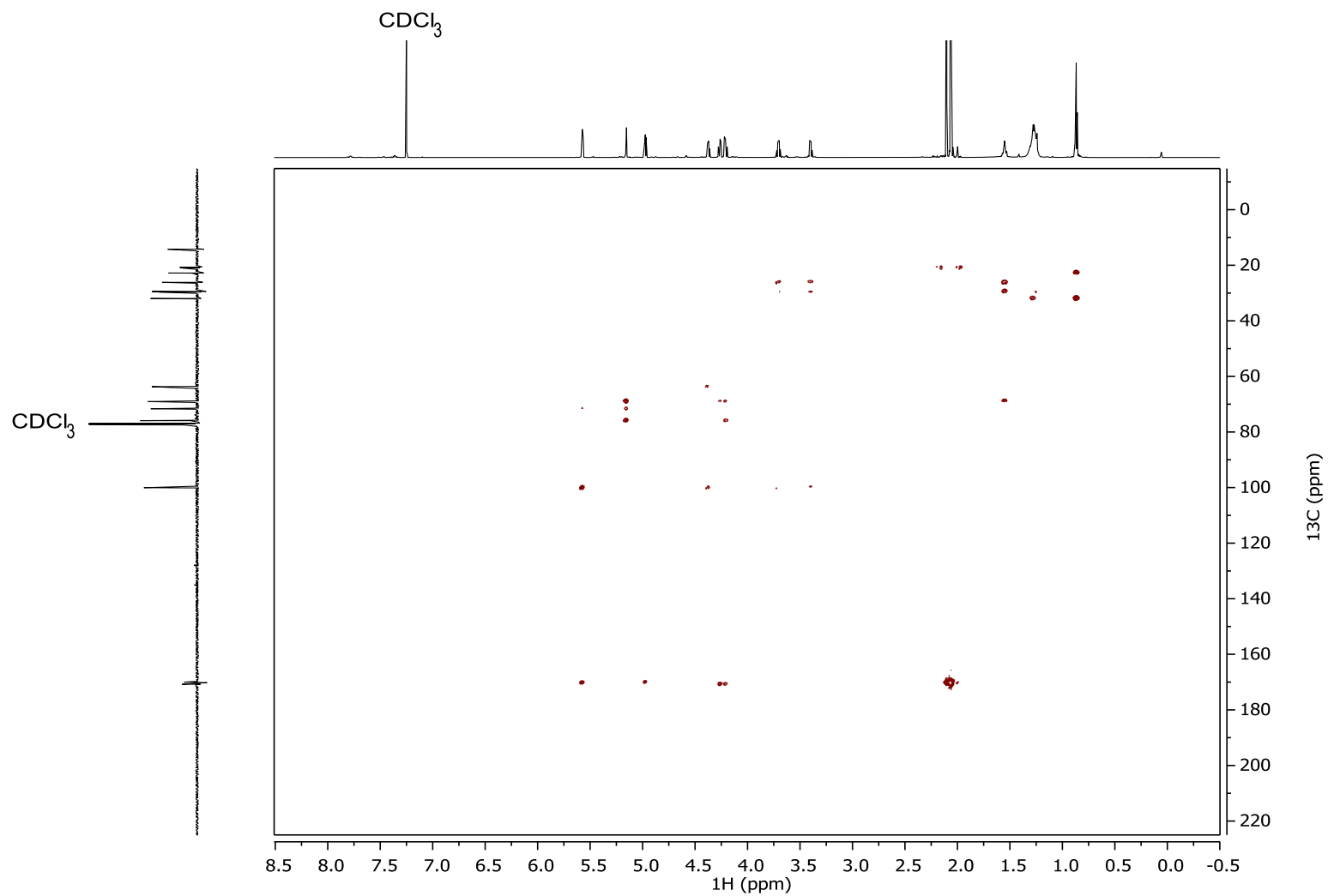
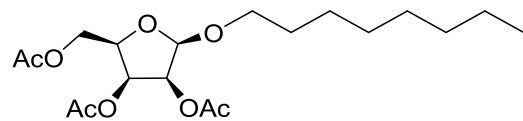
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-lyxofuranoside



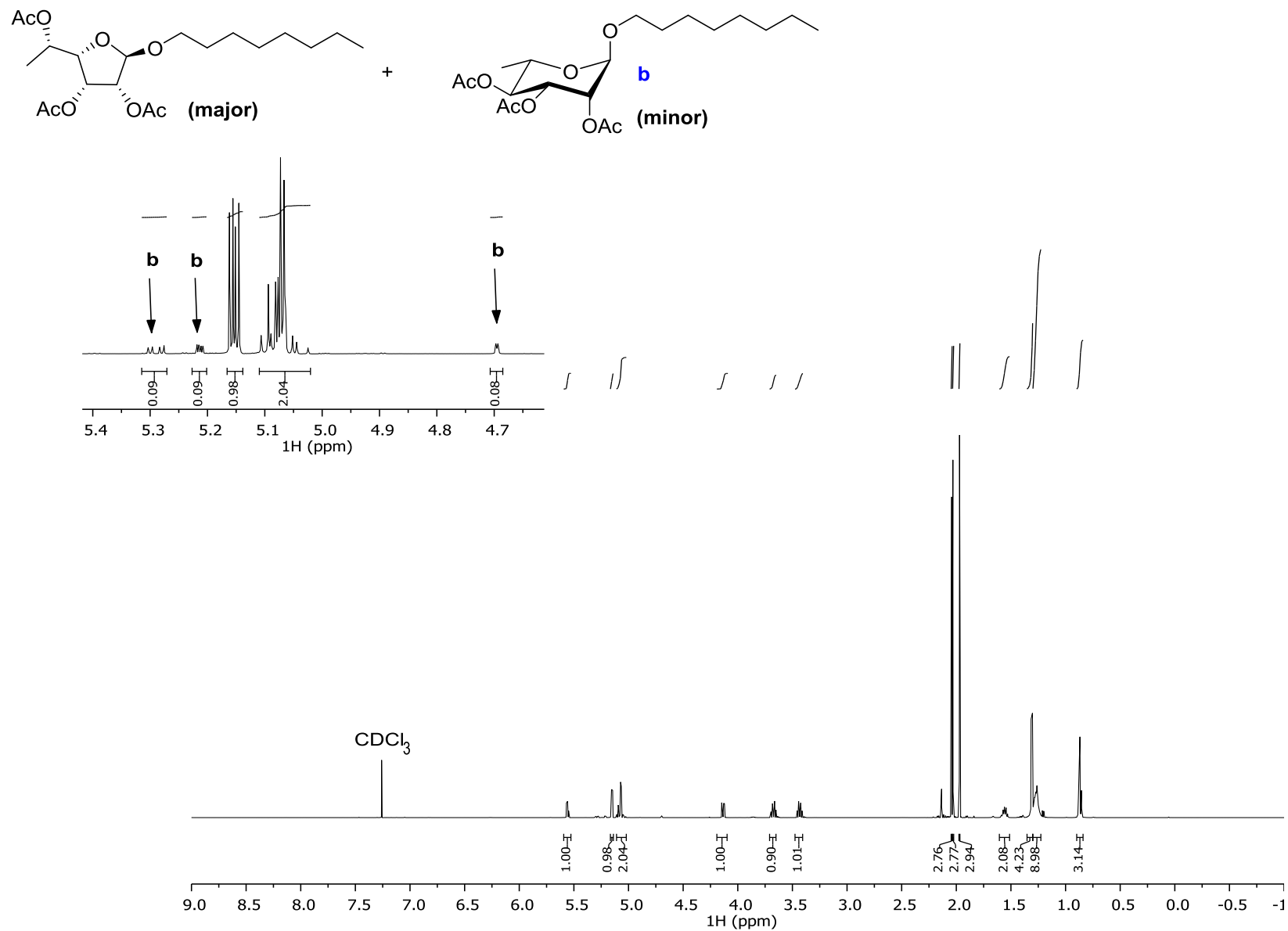
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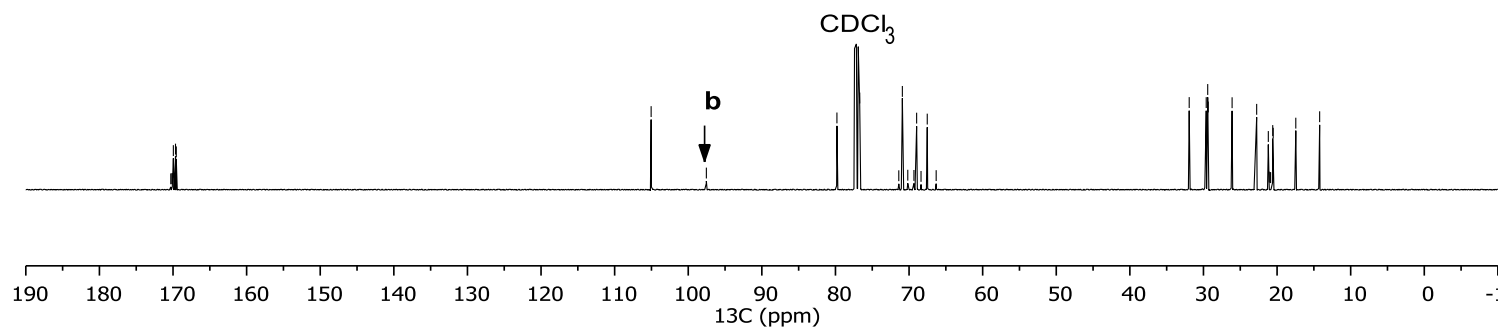
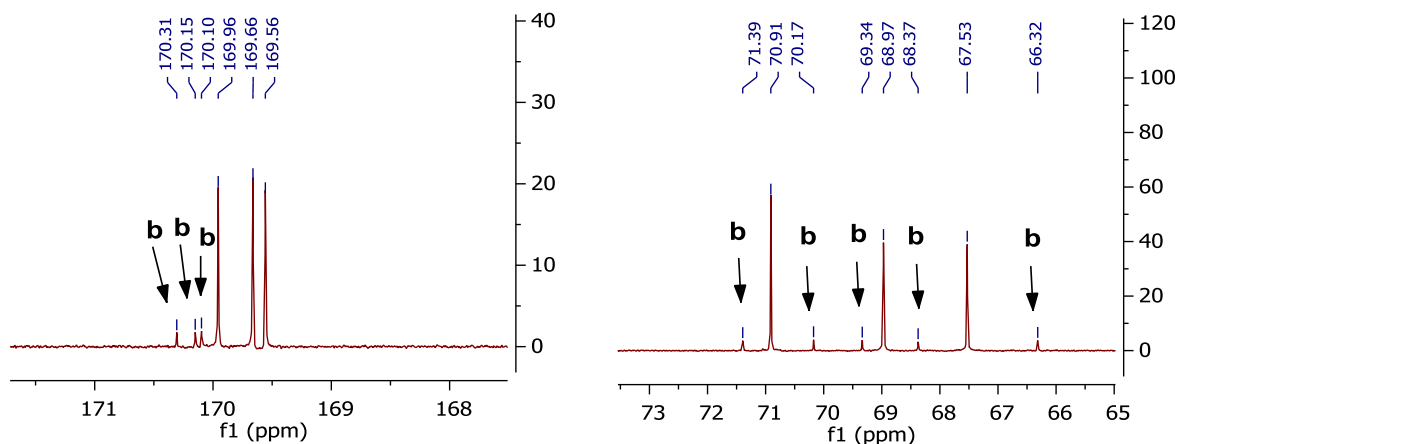
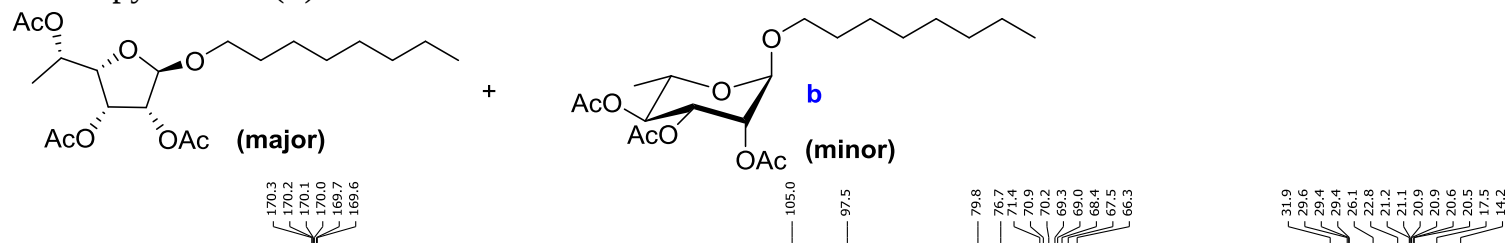
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-lyxofuranoside



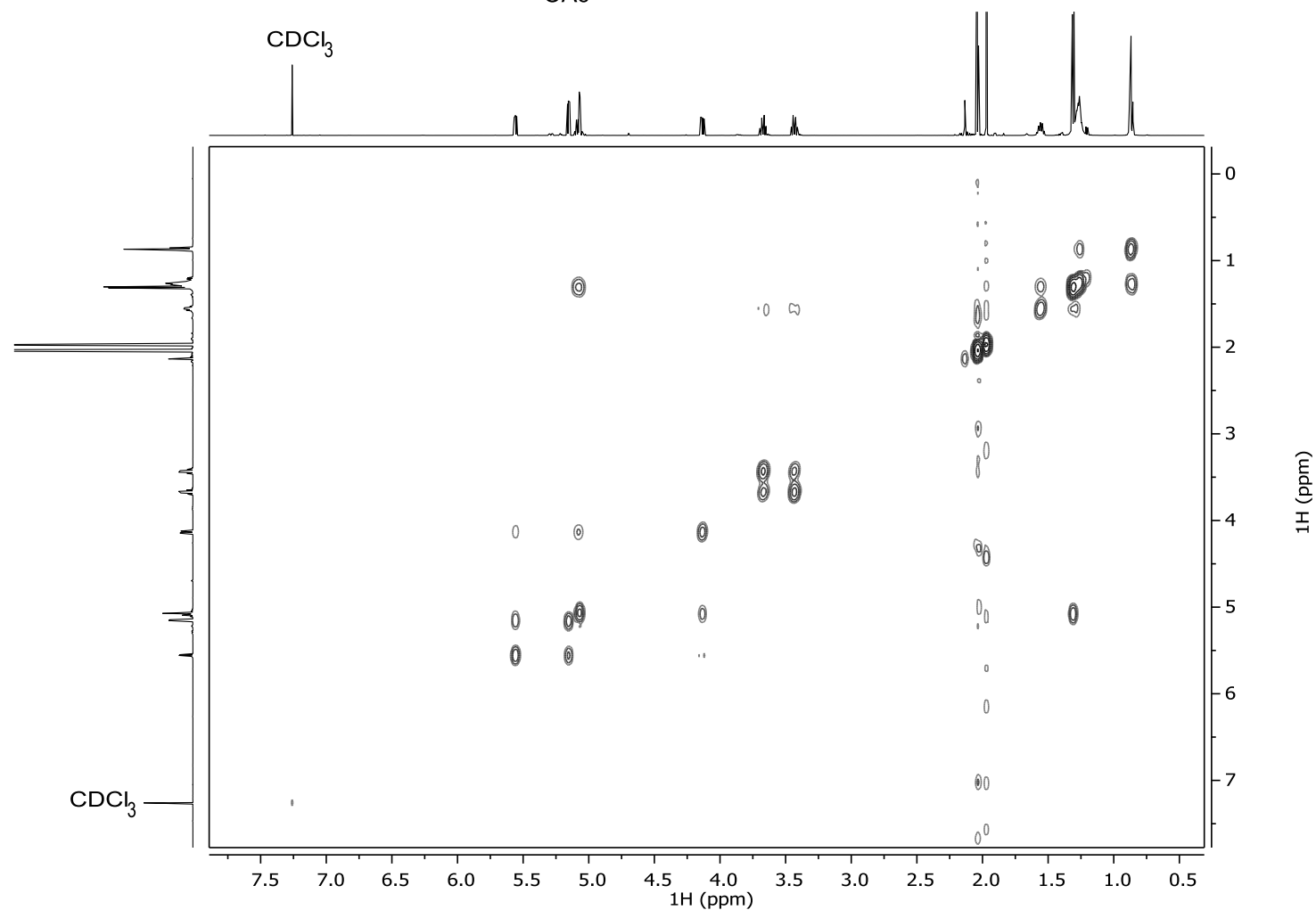
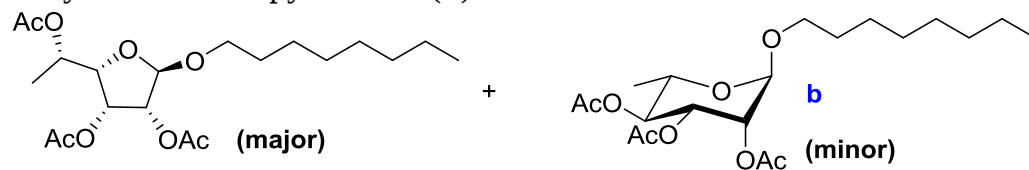
^1H NMR (500 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -L-rhamnofuranoside & *n*-octyl 2,3,4-tri-*O*-acetyl- α -L-rhamnopyranoside (**b**)



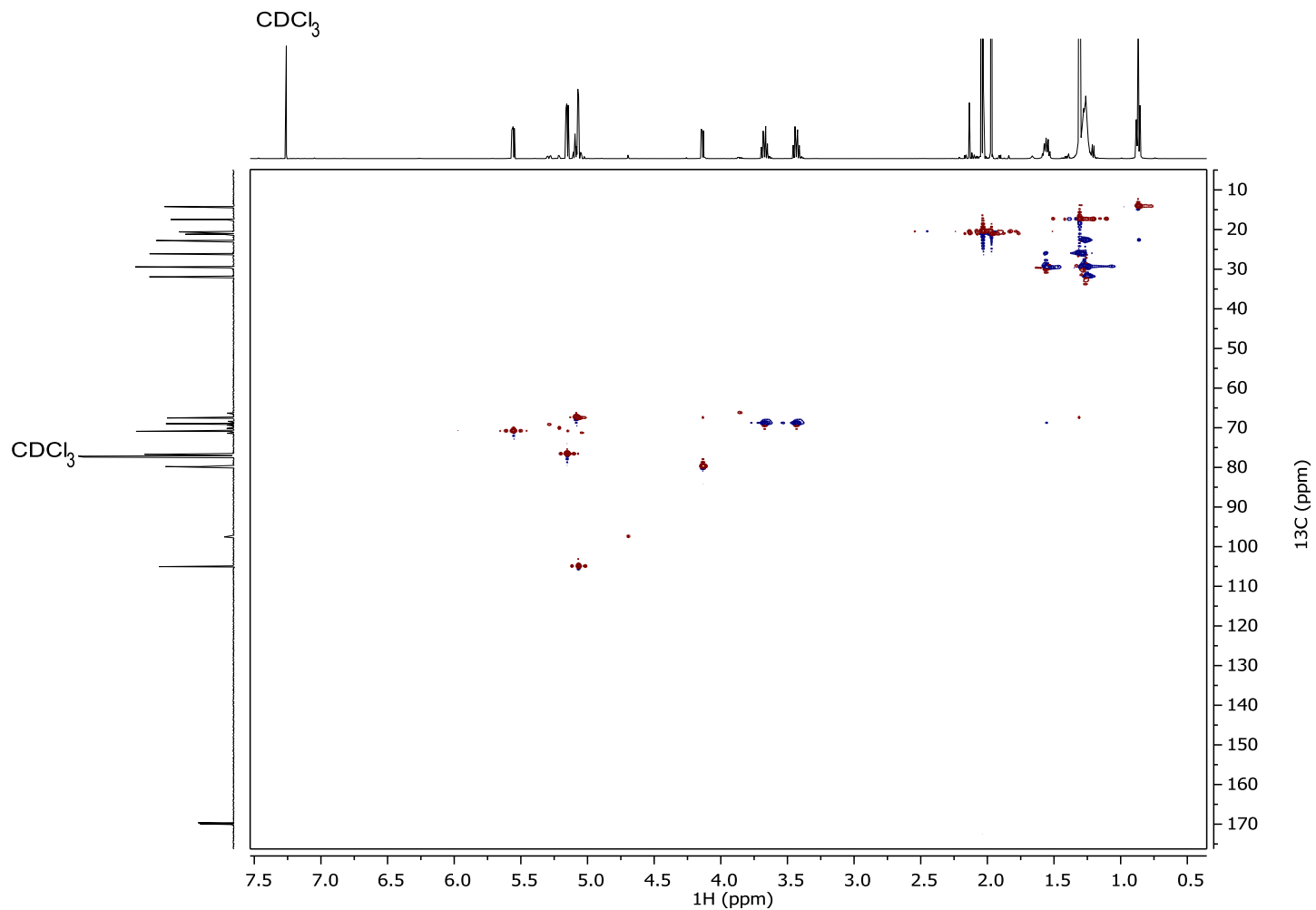
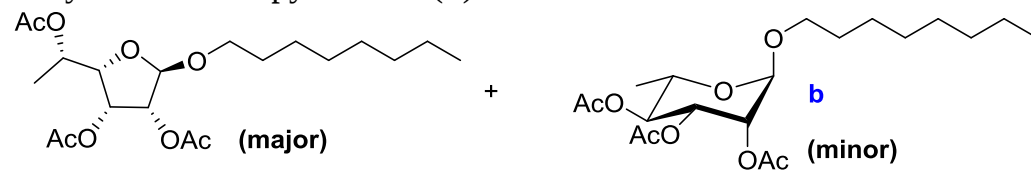
^{13}C NMR (126 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -L-rhamnofuranoside & *n*-octyl 2,3,4-tri-*O*-acetyl- α -L-rhamnopyranoside (**b**)



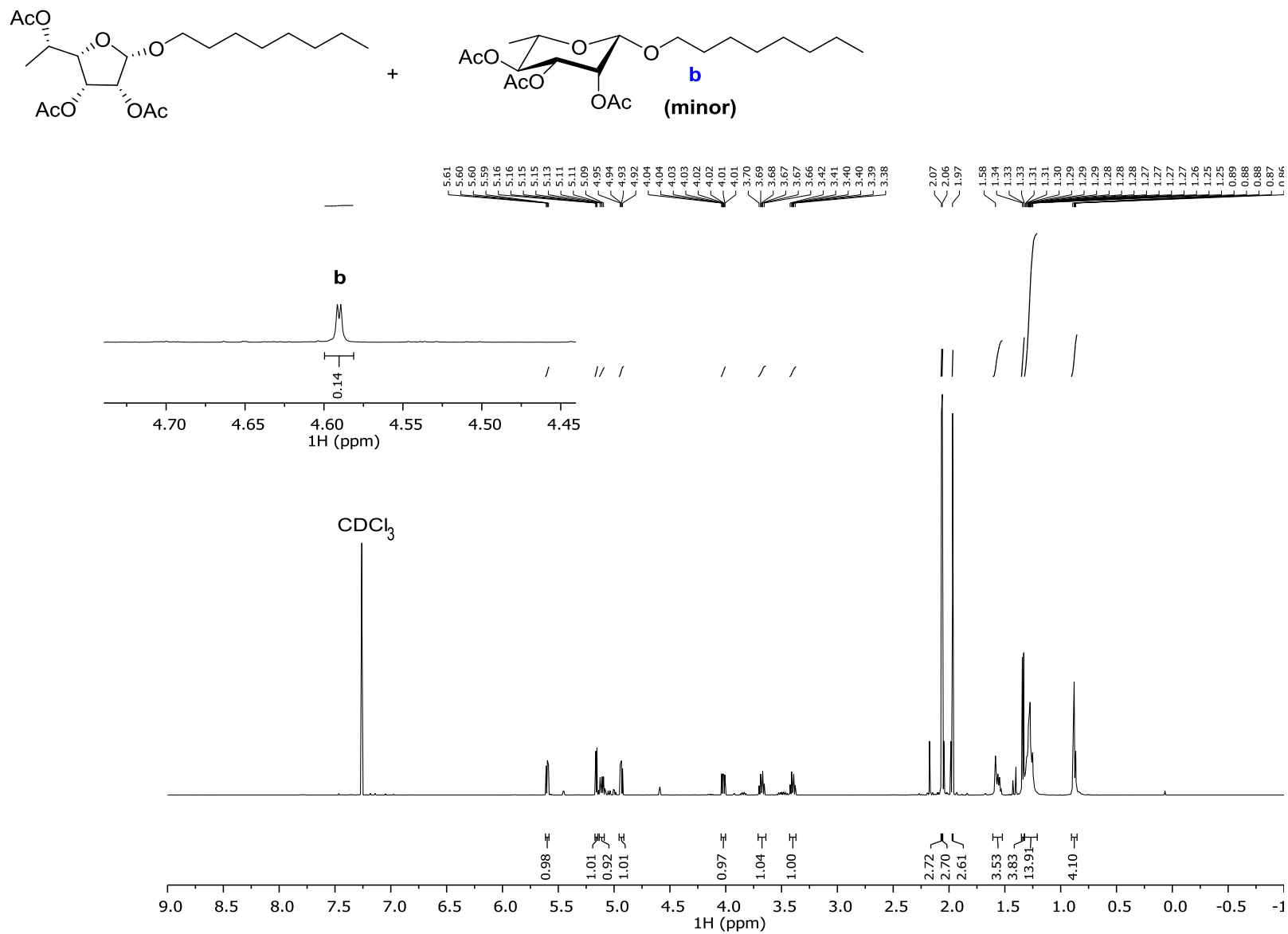
^1H - ^1H COSY NMR (500 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -L-rhamnofuranoside & *n*-octyl 2,3,4-tri-*O*-acetyl- α -L-rhamnopyranoside (**b**)



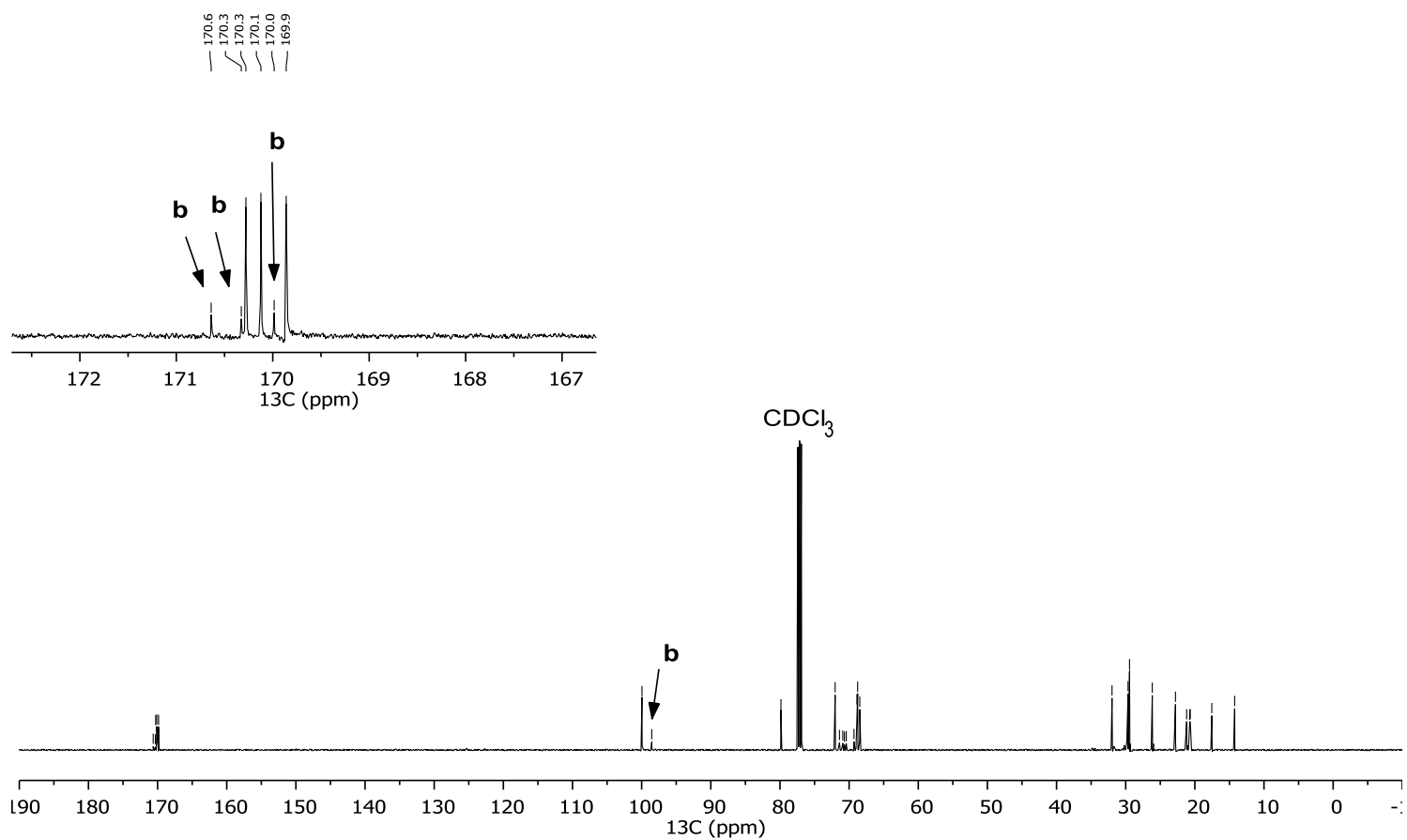
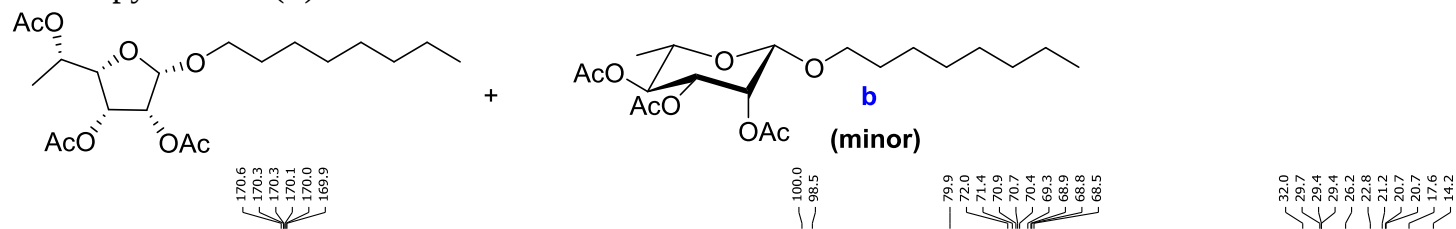
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -L-rhamnofuranoside & *n*-octyl 2,3,4-tri-*O*-acetyl- α -L-rhamnopyranoside (b**)**



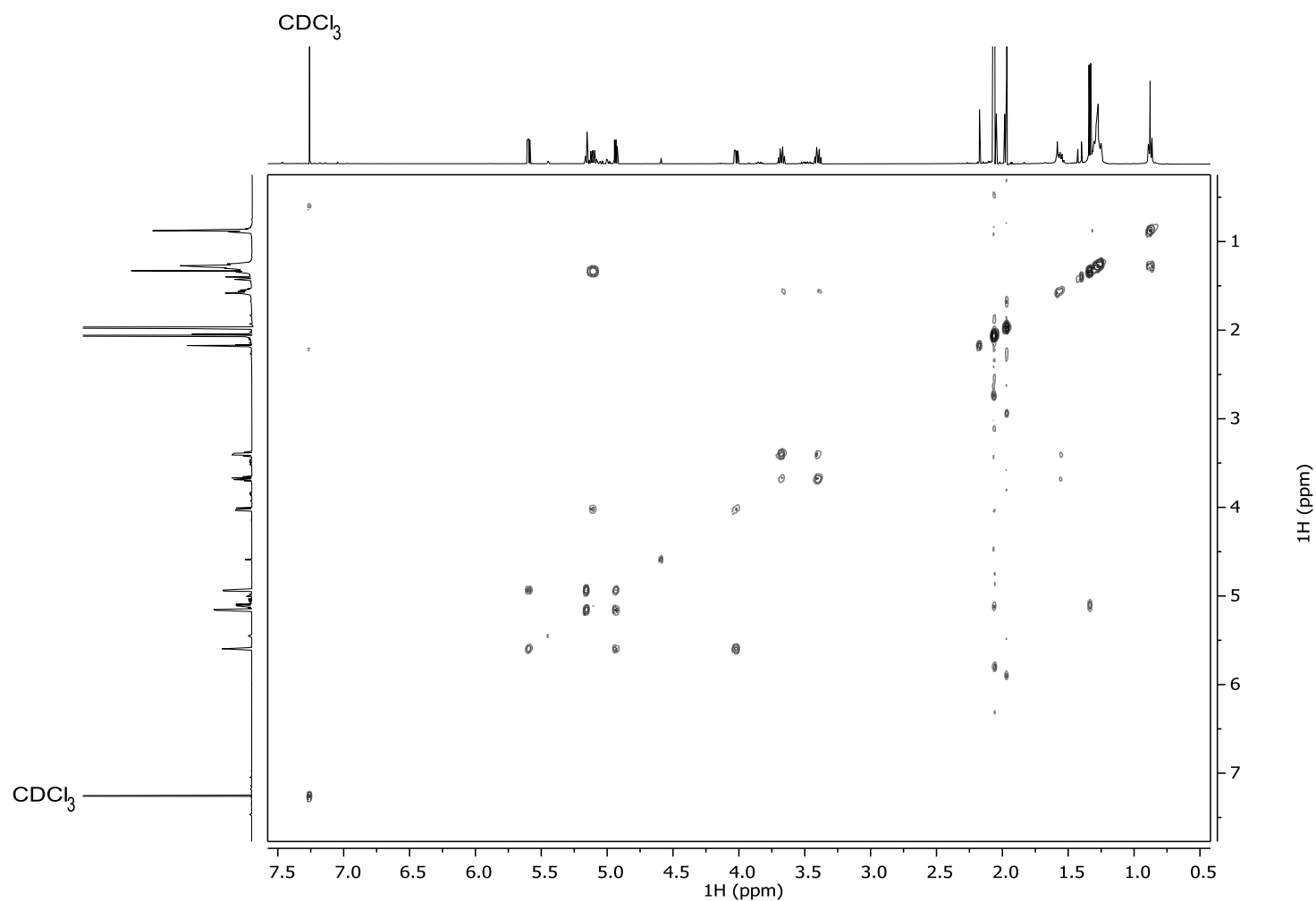
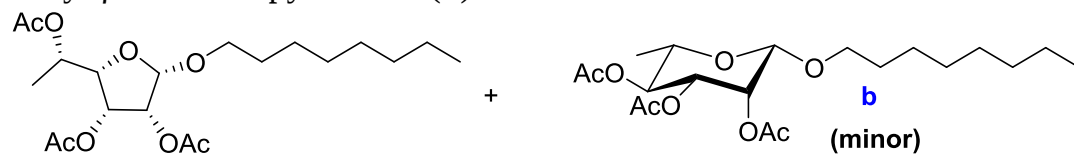
^1H NMR (500 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- β -L-rhamnofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -L-rhamnopyranoside (**b**)



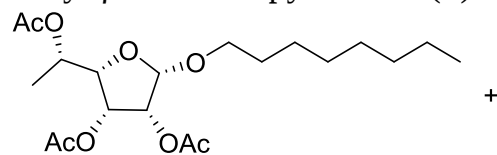
^{13}C NMR (126 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- β -L-rhamnofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -L-rhamnopyranoside (**b**)



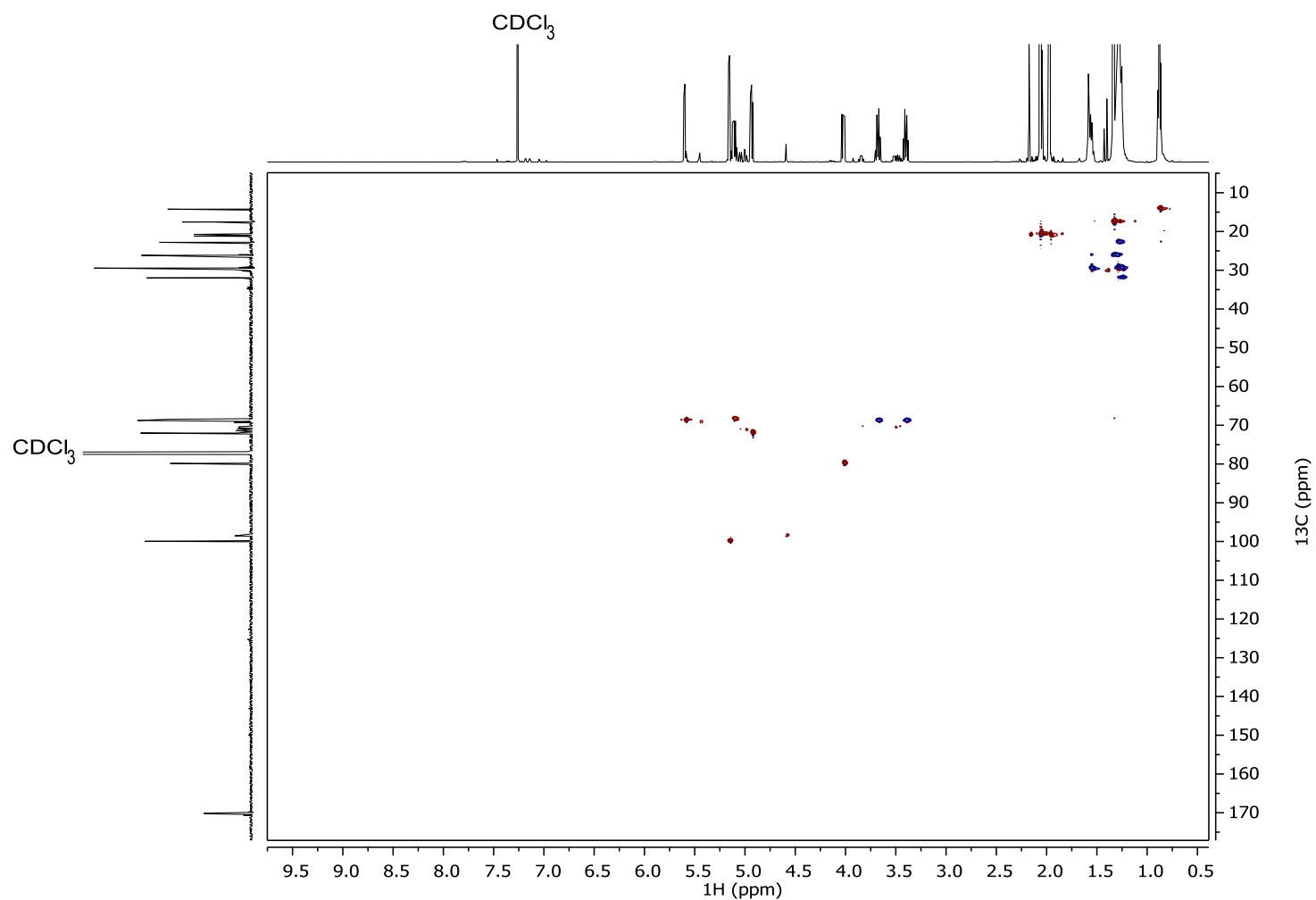
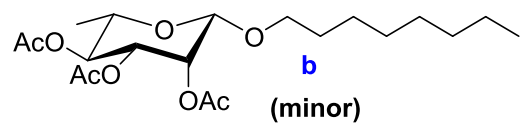
^1H - ^1H COSY NMR (500 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- β -L-rhamnofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -L-rhamnopyranoside (**b**)



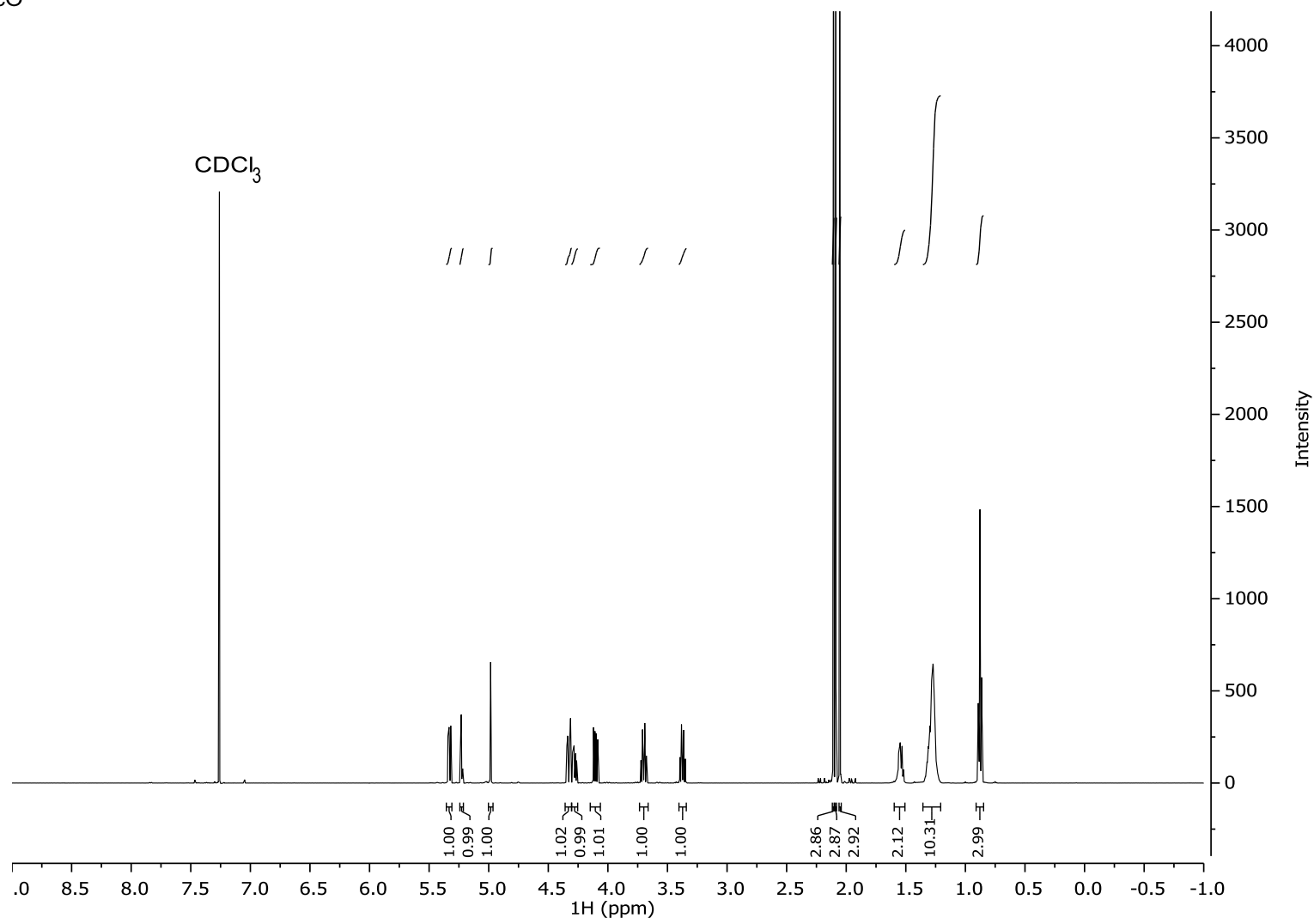
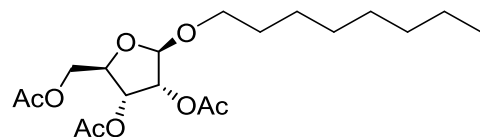
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- β -L-rhamnofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -L-rhamnopyranoside (**b**)



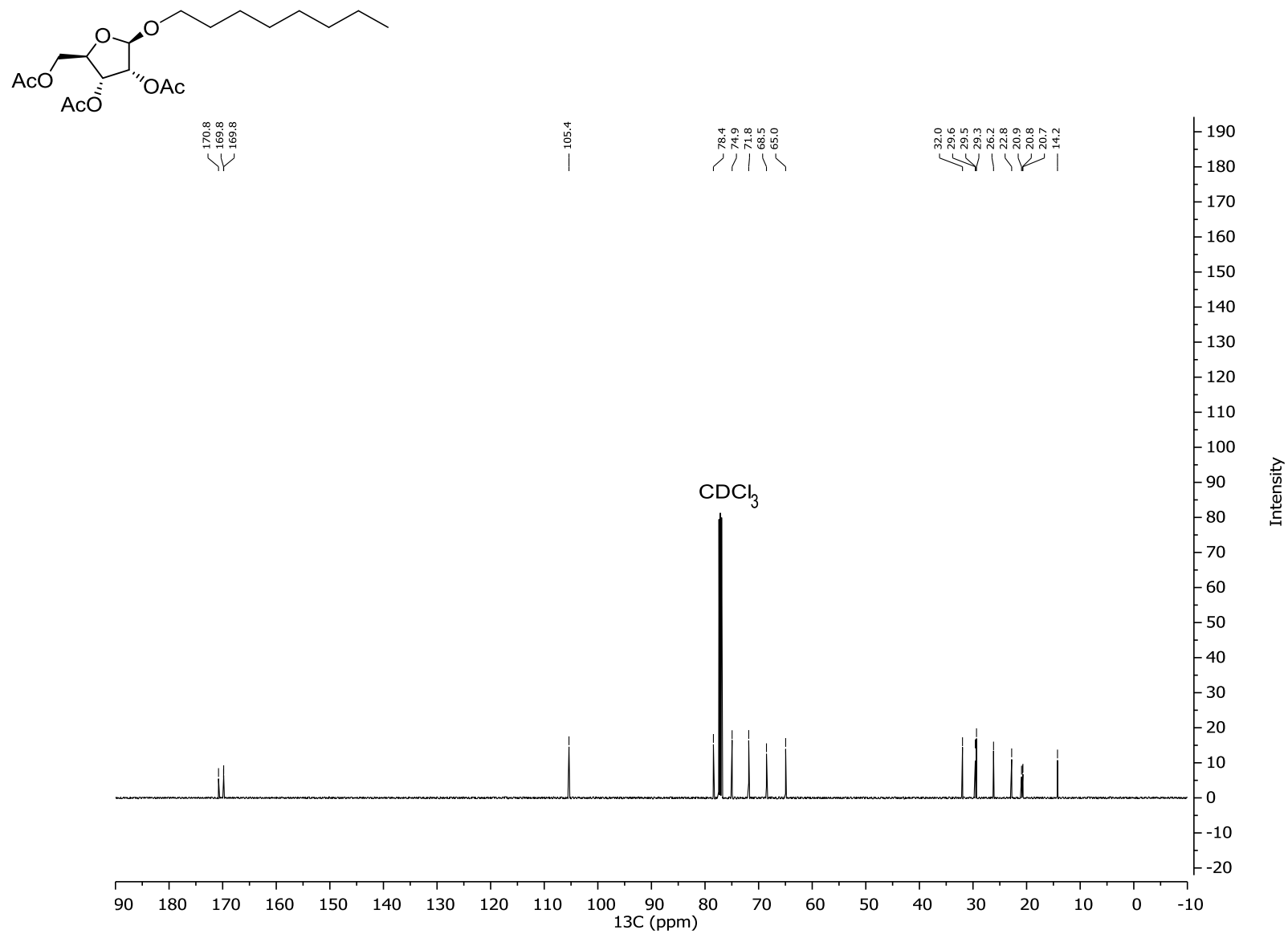
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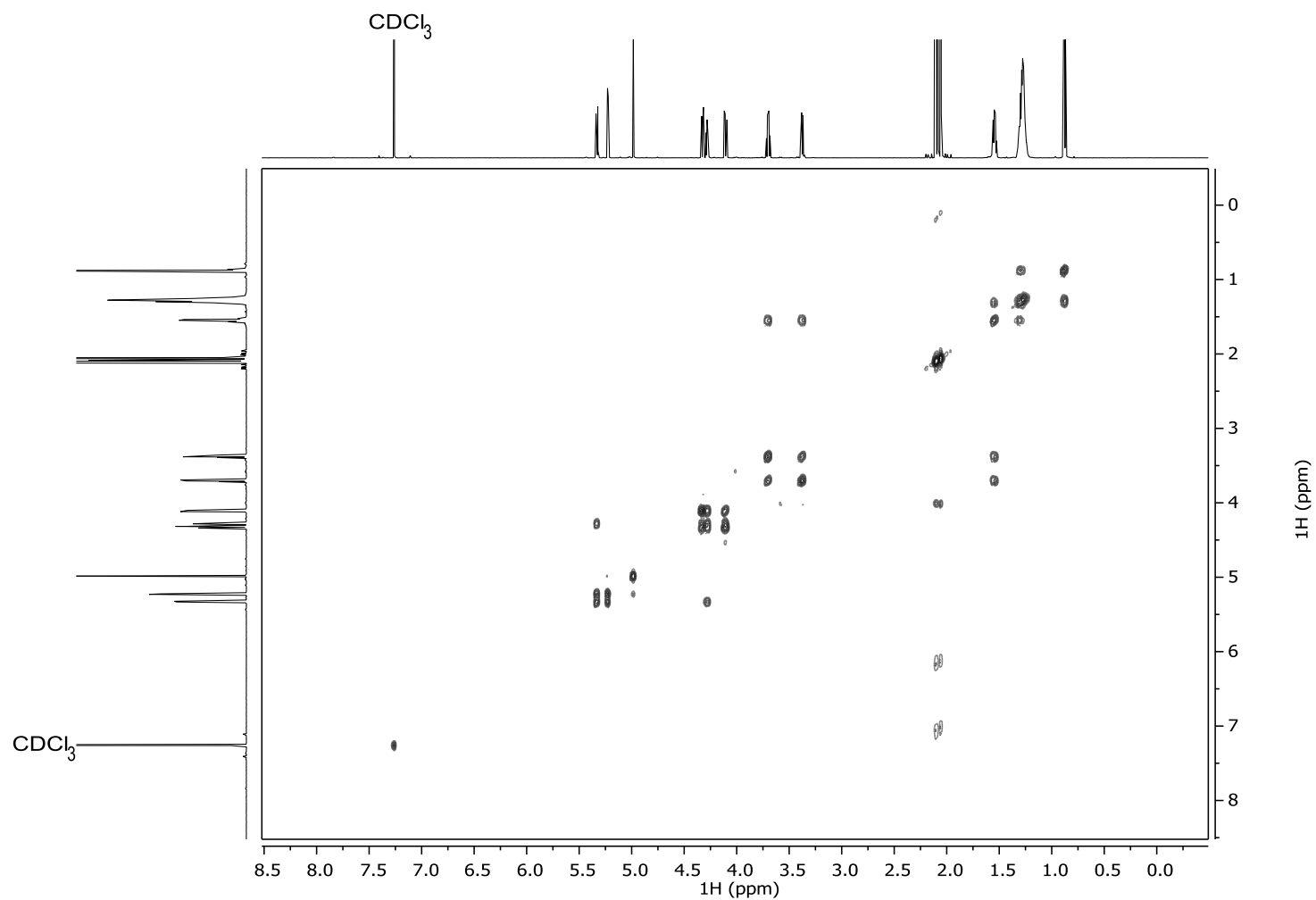
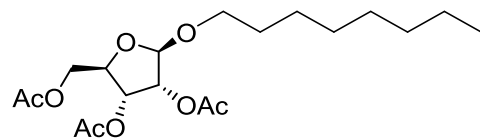
¹H NMR (500 MHz, CDCl₃) *n*-octyl 2,3,5-tri-*O*-acetyl-β-D-ribofuranoside



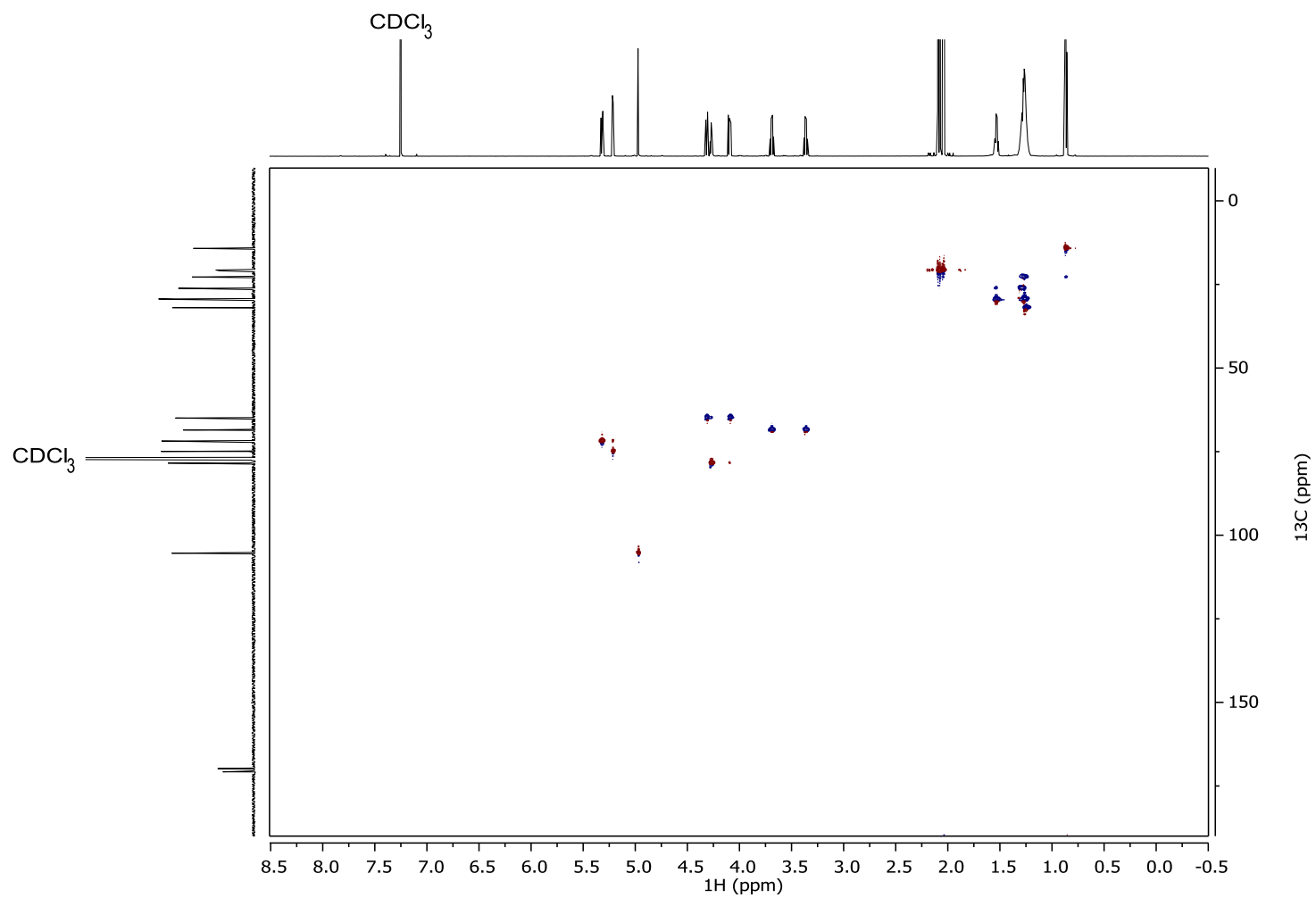
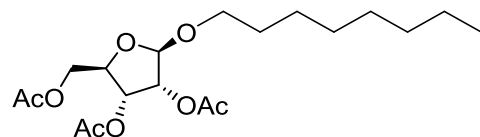
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-ribofuranoside



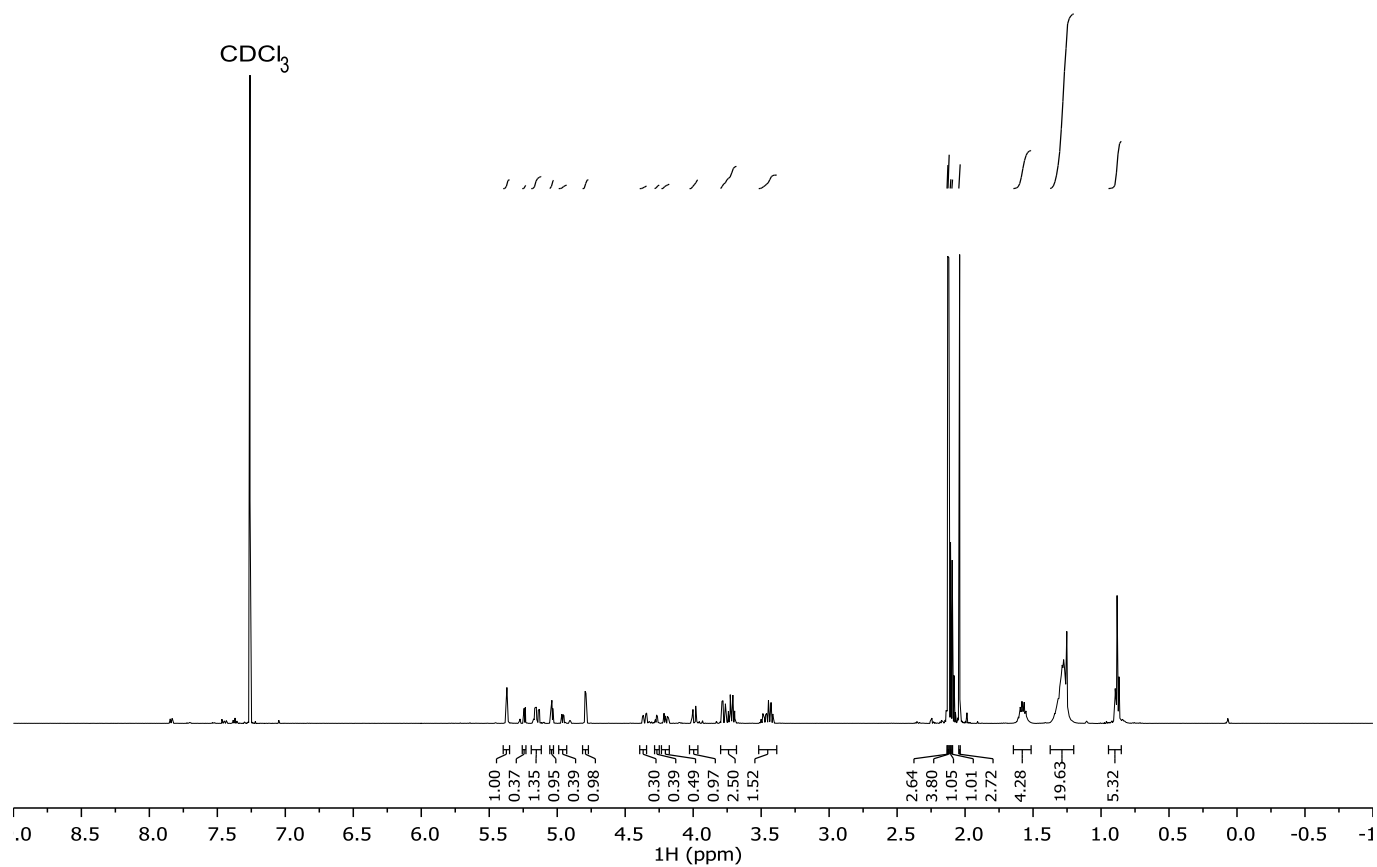
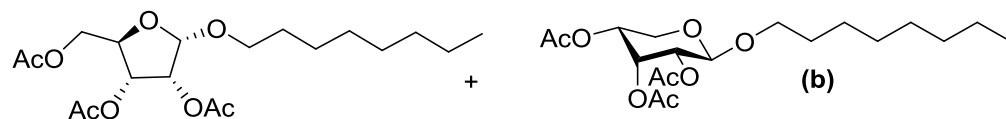
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-ribofuranoside



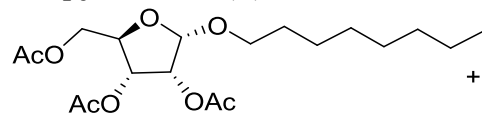
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-ribofuranoside



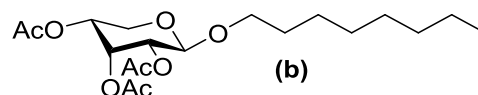
¹H NMR (500 MHz, CDCl₃) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-ribofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-ribofuranoside **(b)**



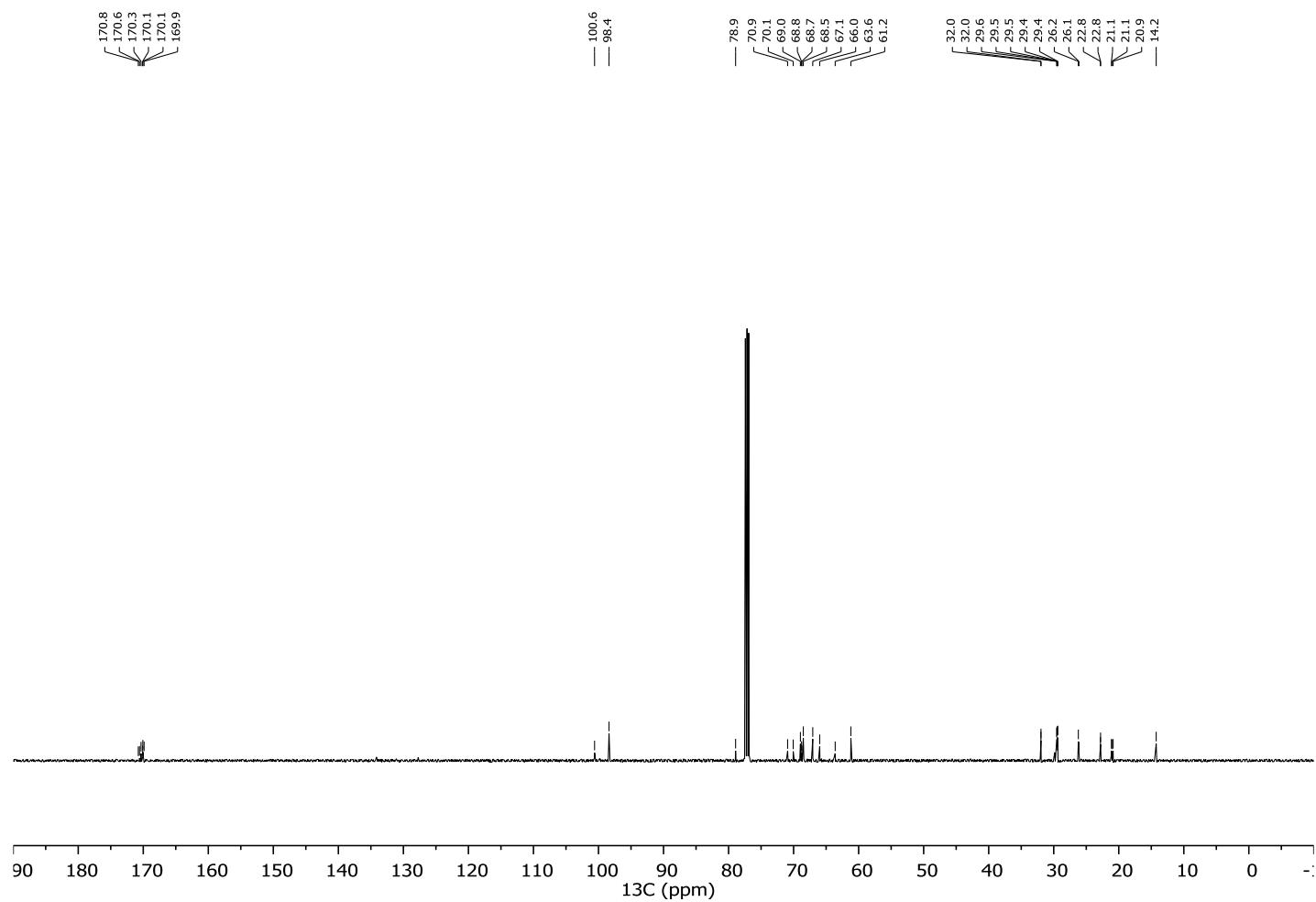
^{13}C NMR (126 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-ribofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-ribofuranoside **(b)**



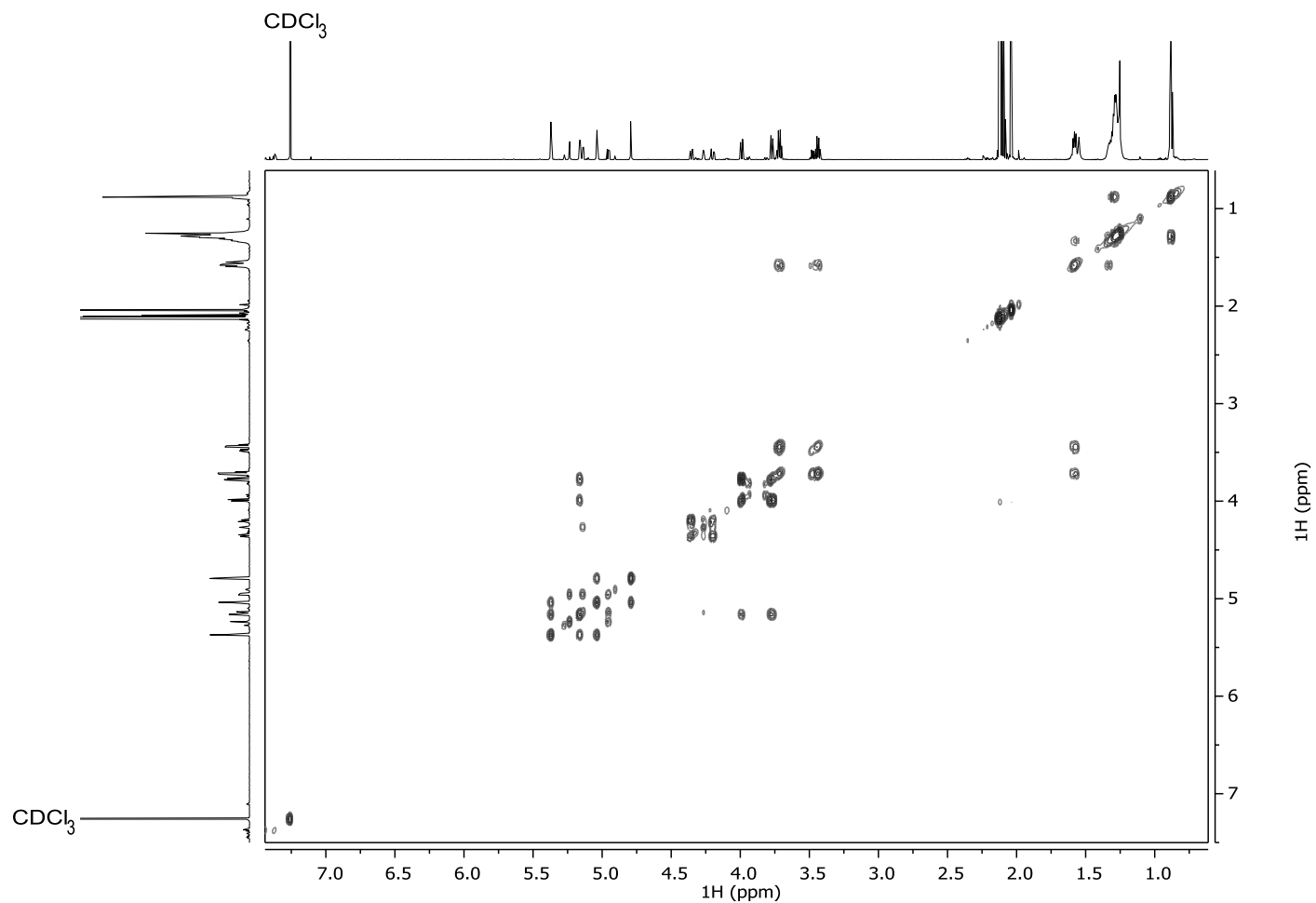
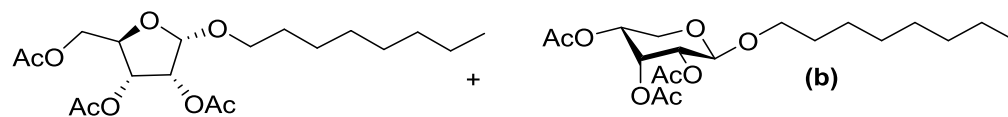
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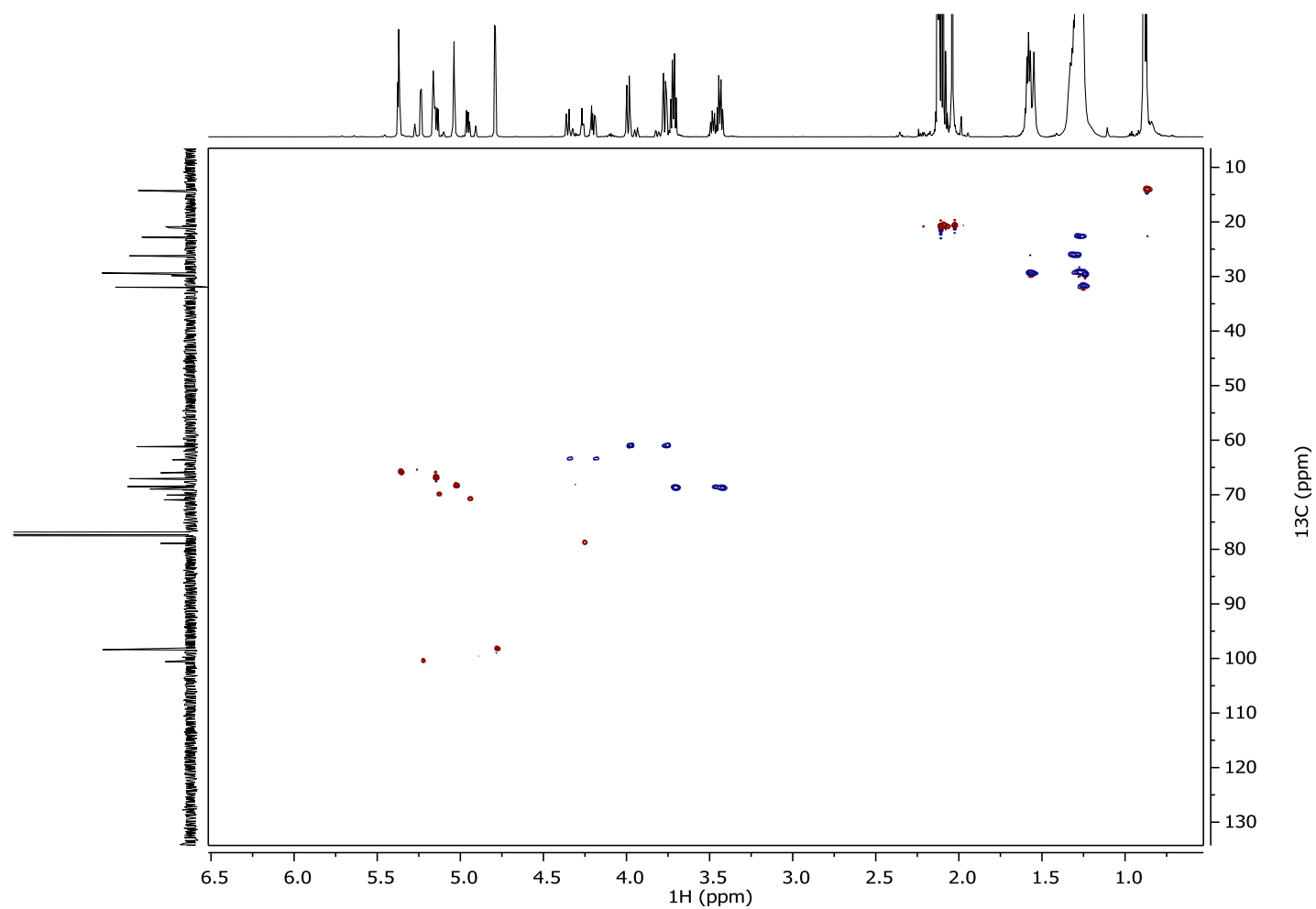
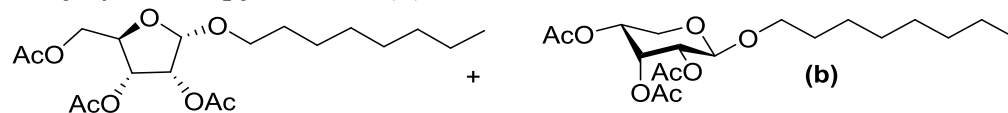
(b)



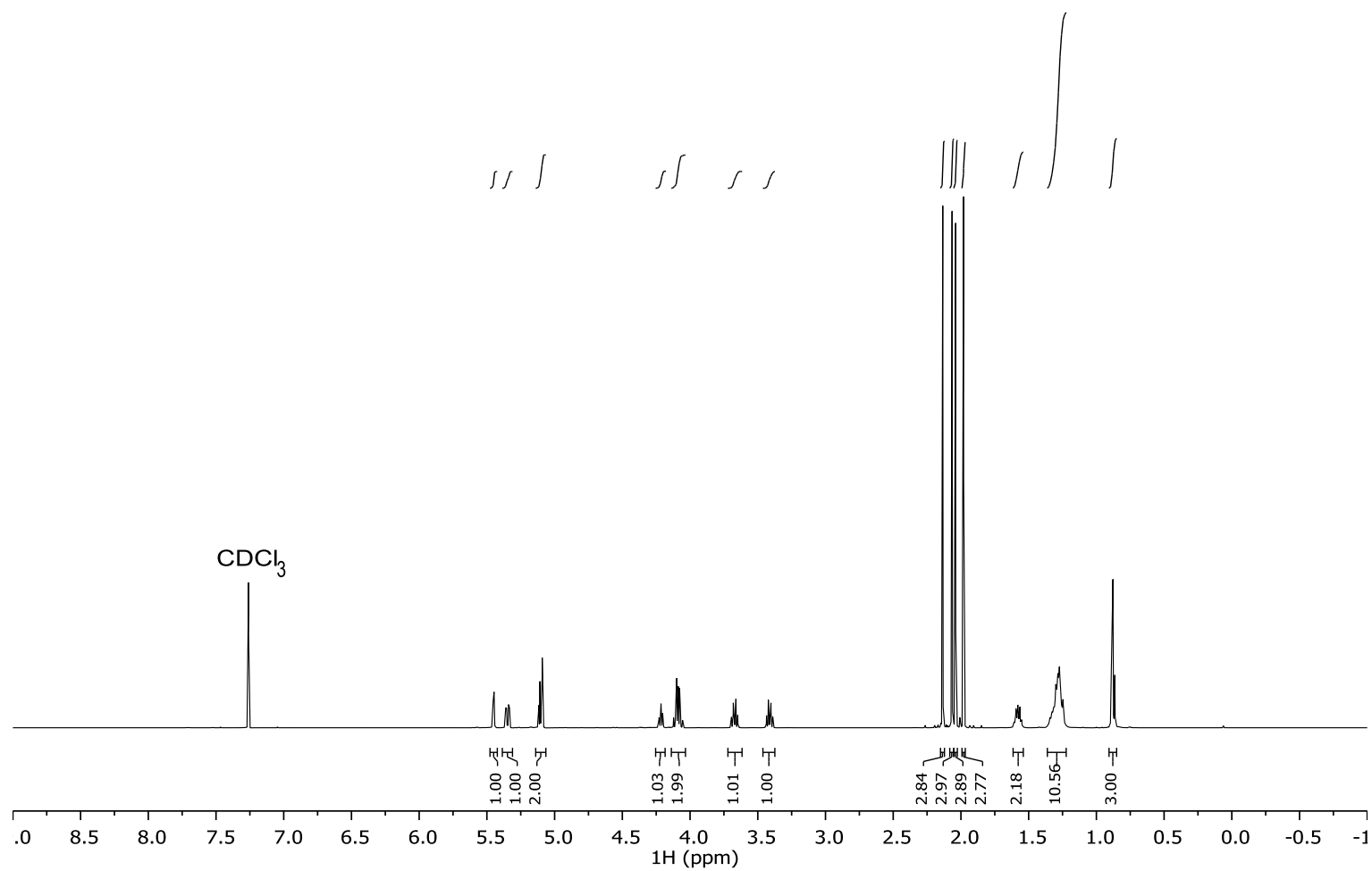
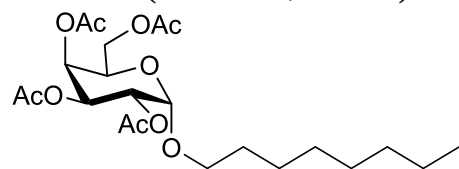
^1H - ^1H COSY NMR (700 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-ribofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-ribofuranoside **(b)**



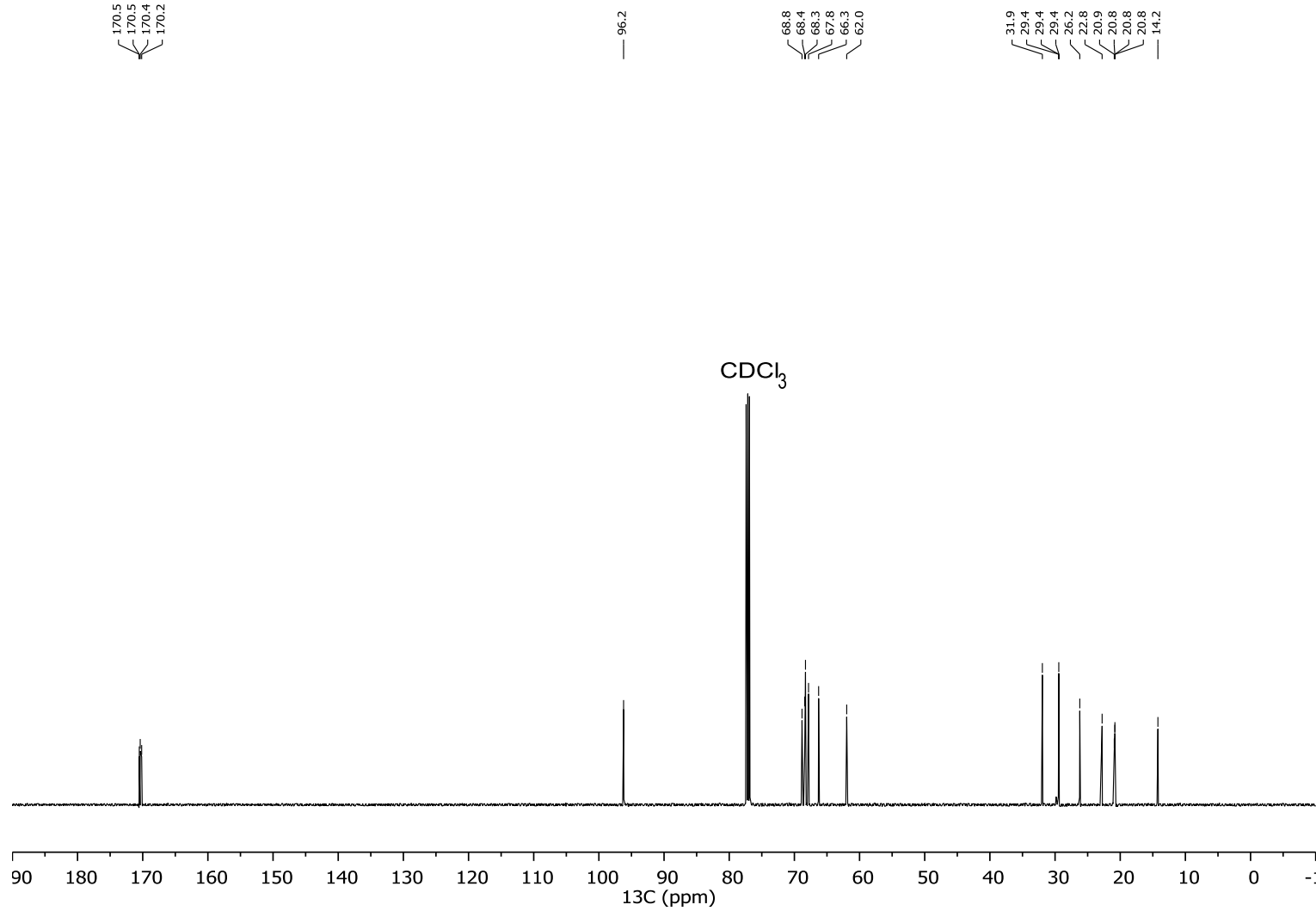
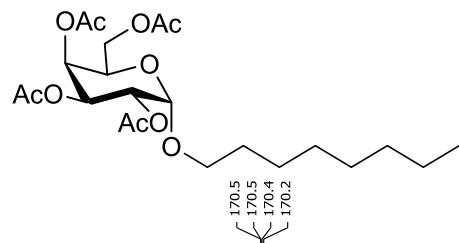
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) Mixture of *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-ribofuranoside + *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-ribofuranoside (b)



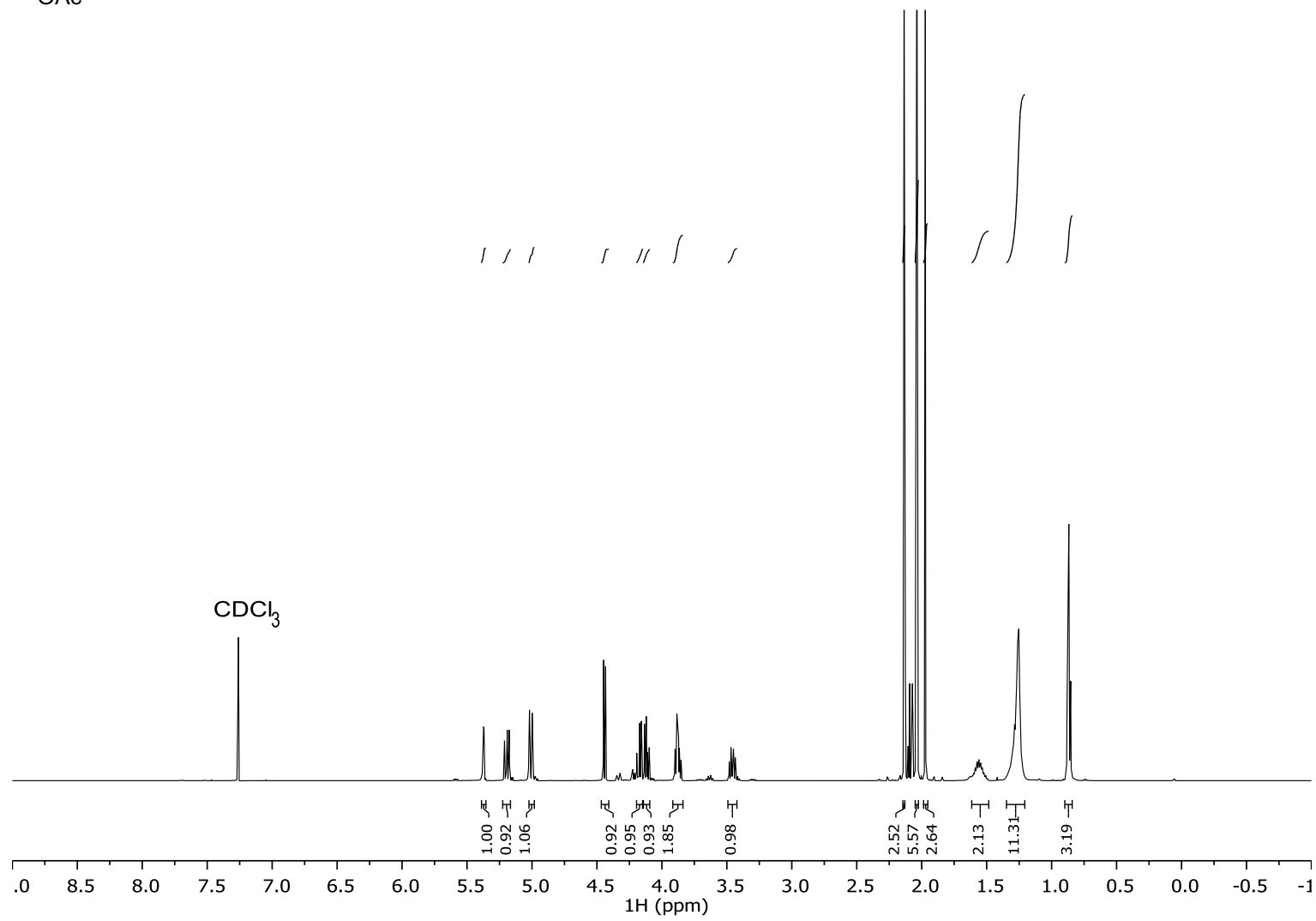
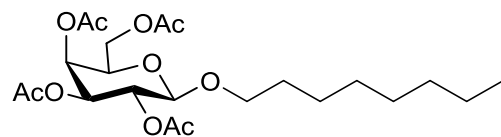
¹H NMR (500 MHz, CDCl₃) n-octyl 2,3,4,6-tetra-O-acetyl- α -D-galactopyranoside



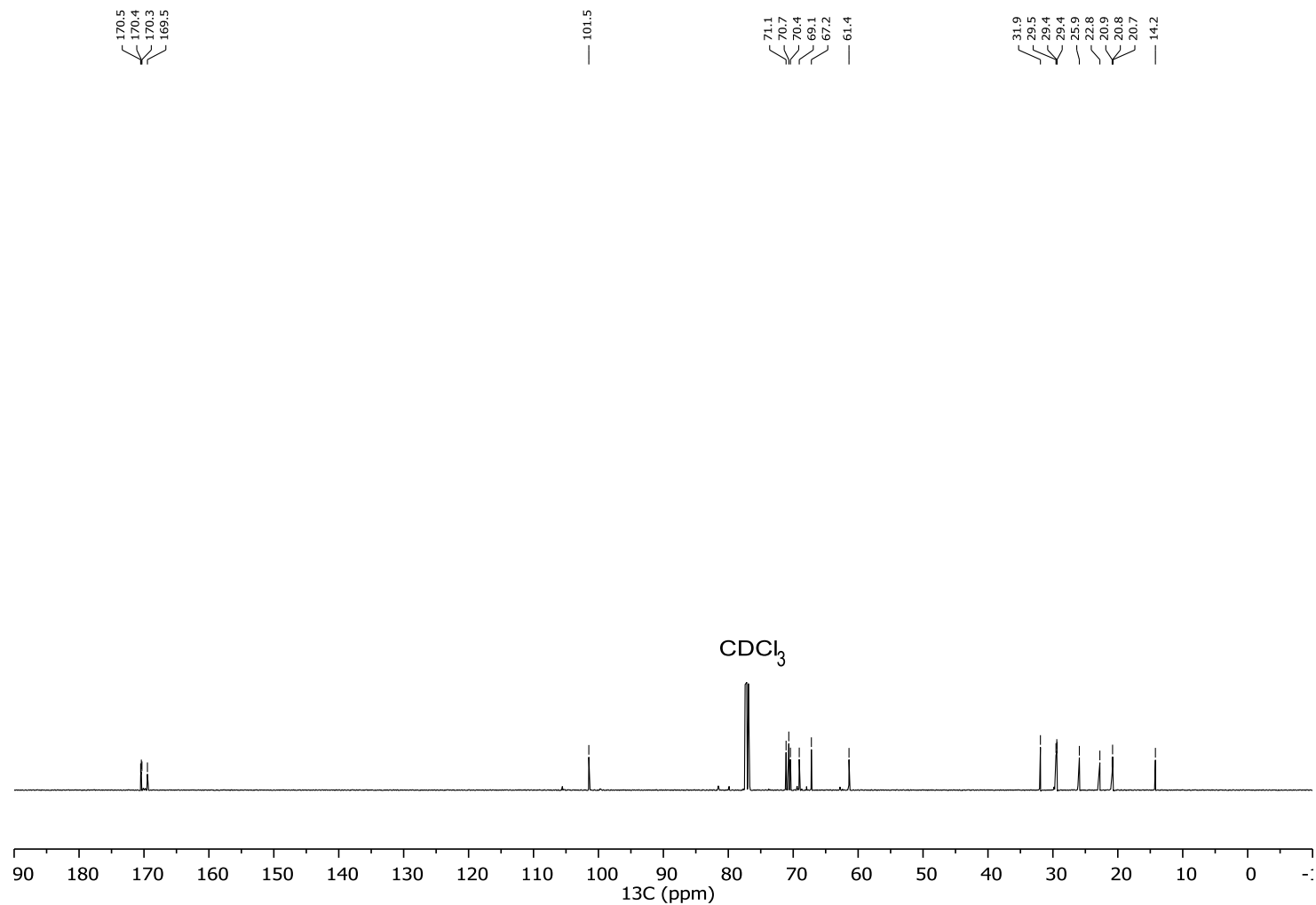
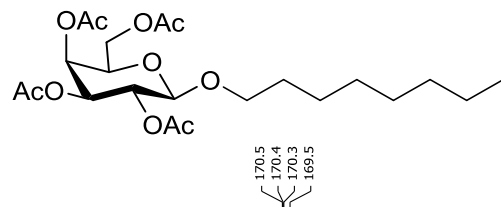
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,4,6-tetra-*O*-acetyl- α -D-galactopyranoside



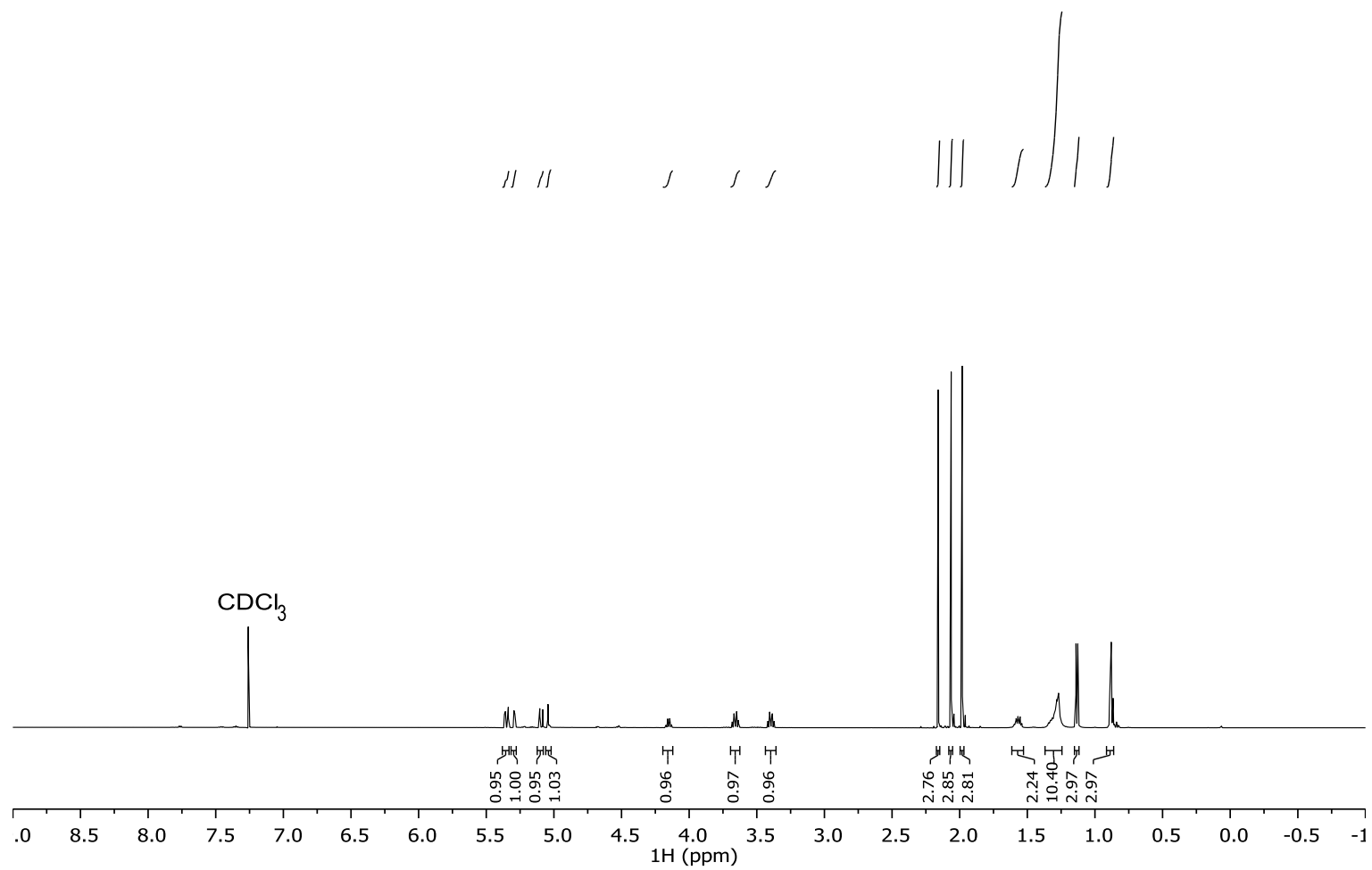
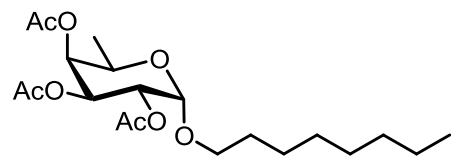
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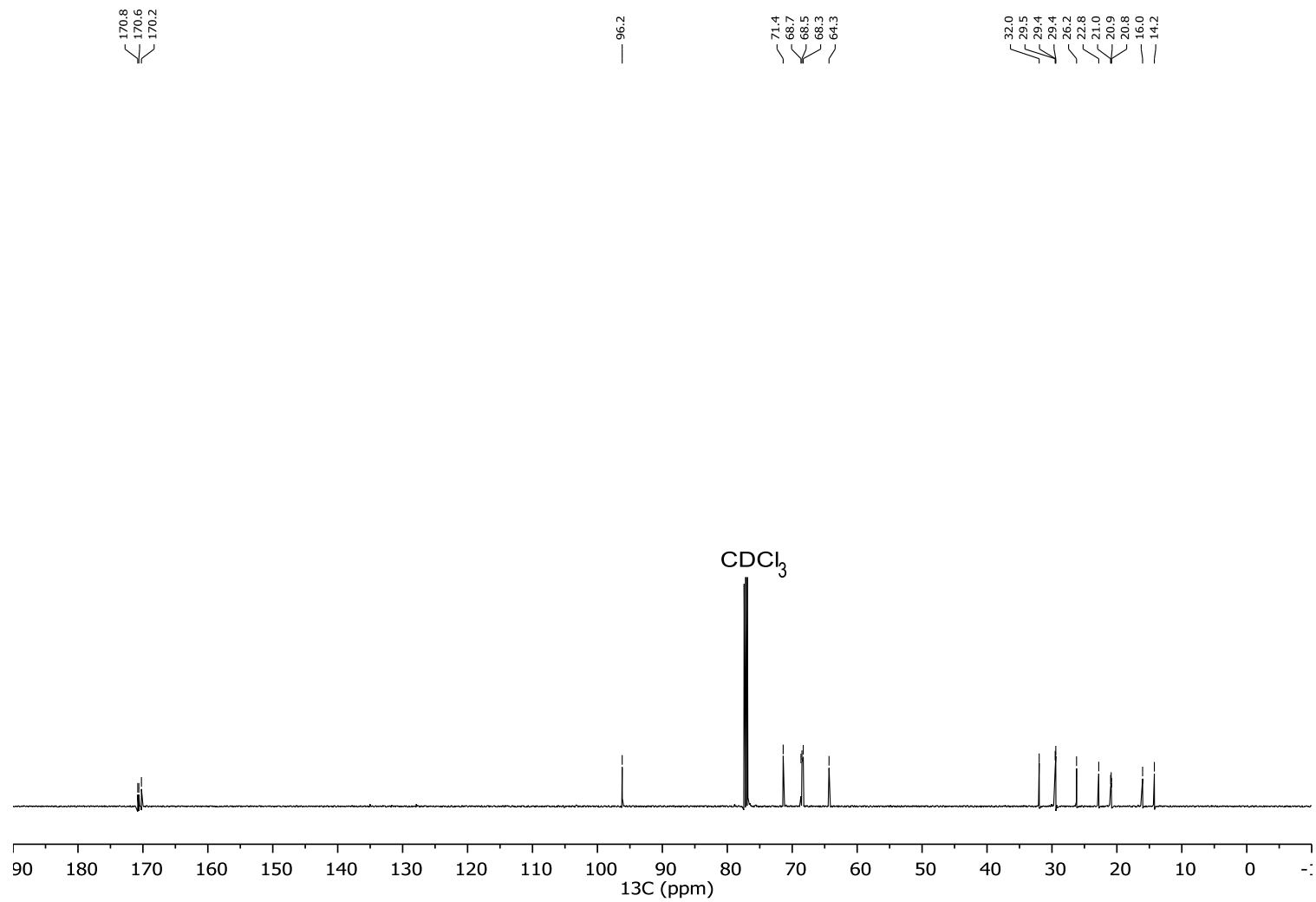
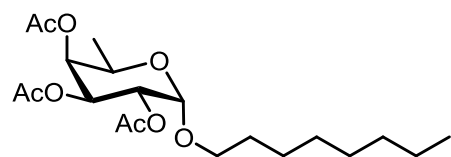
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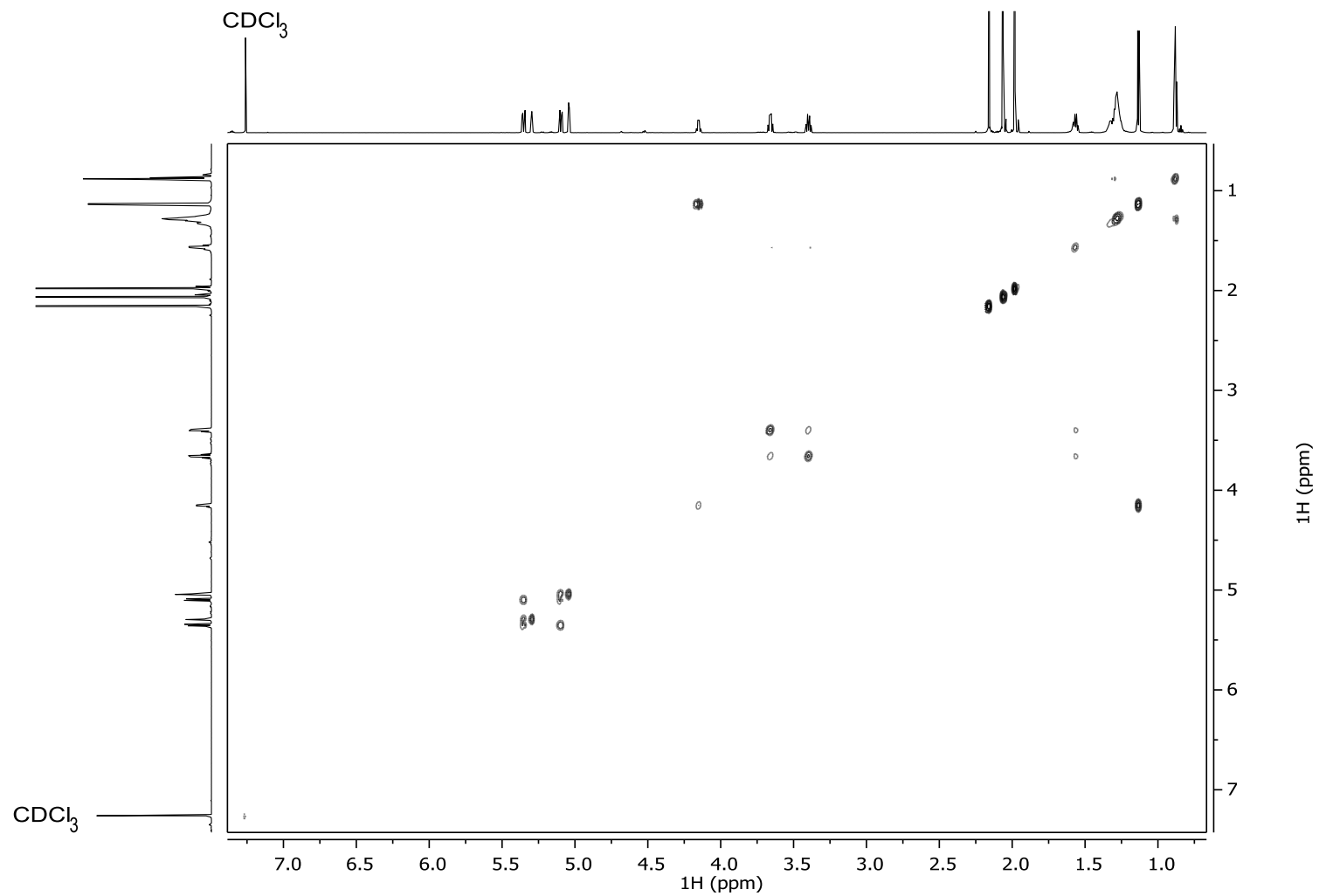
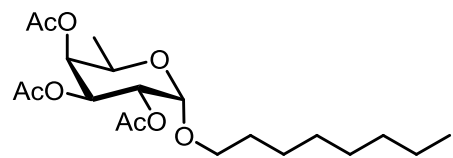
^1H NMR (500 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-fucopyranoside



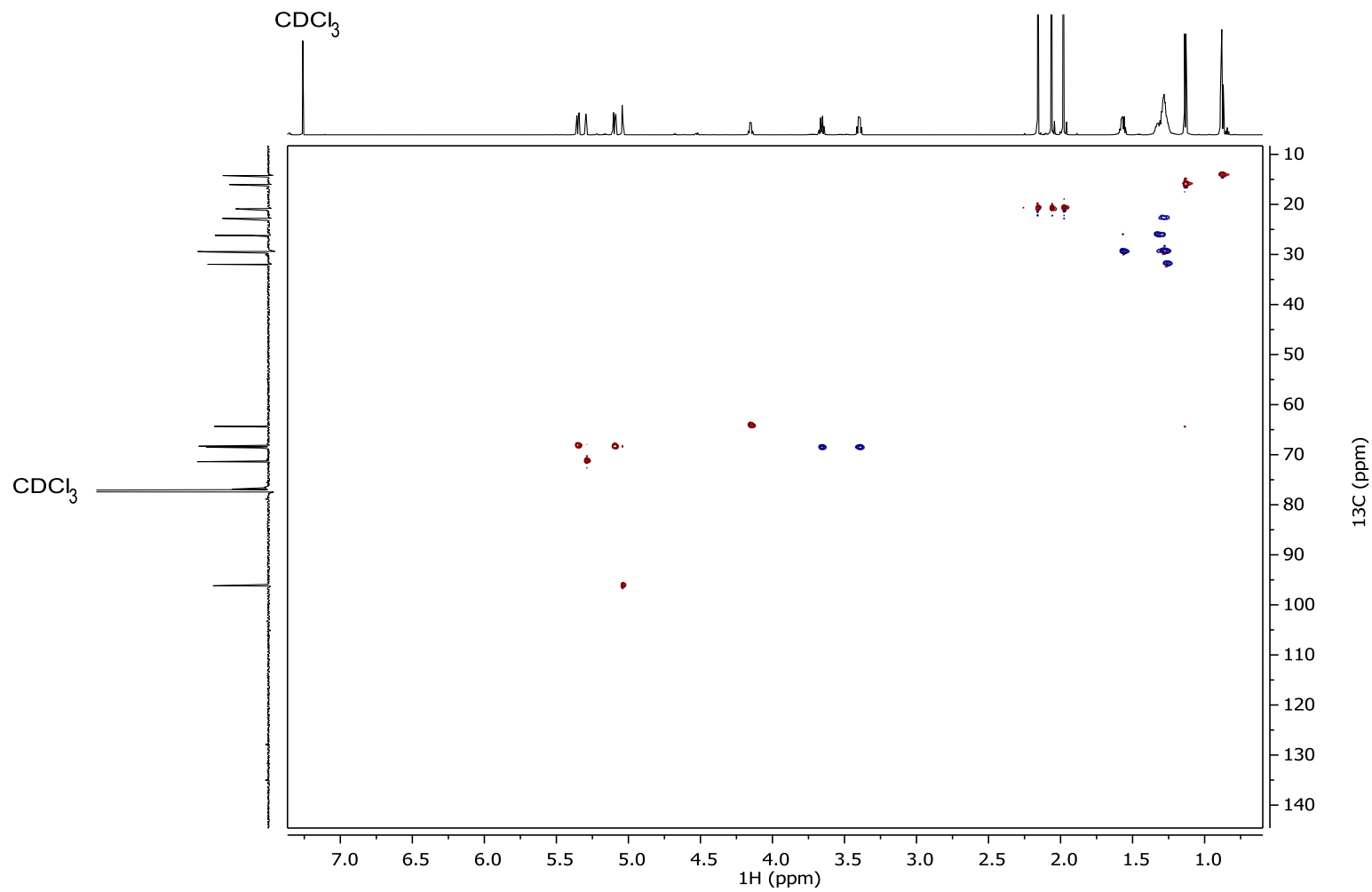
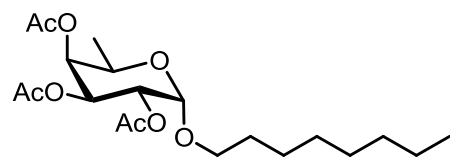
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-fucopyranoside



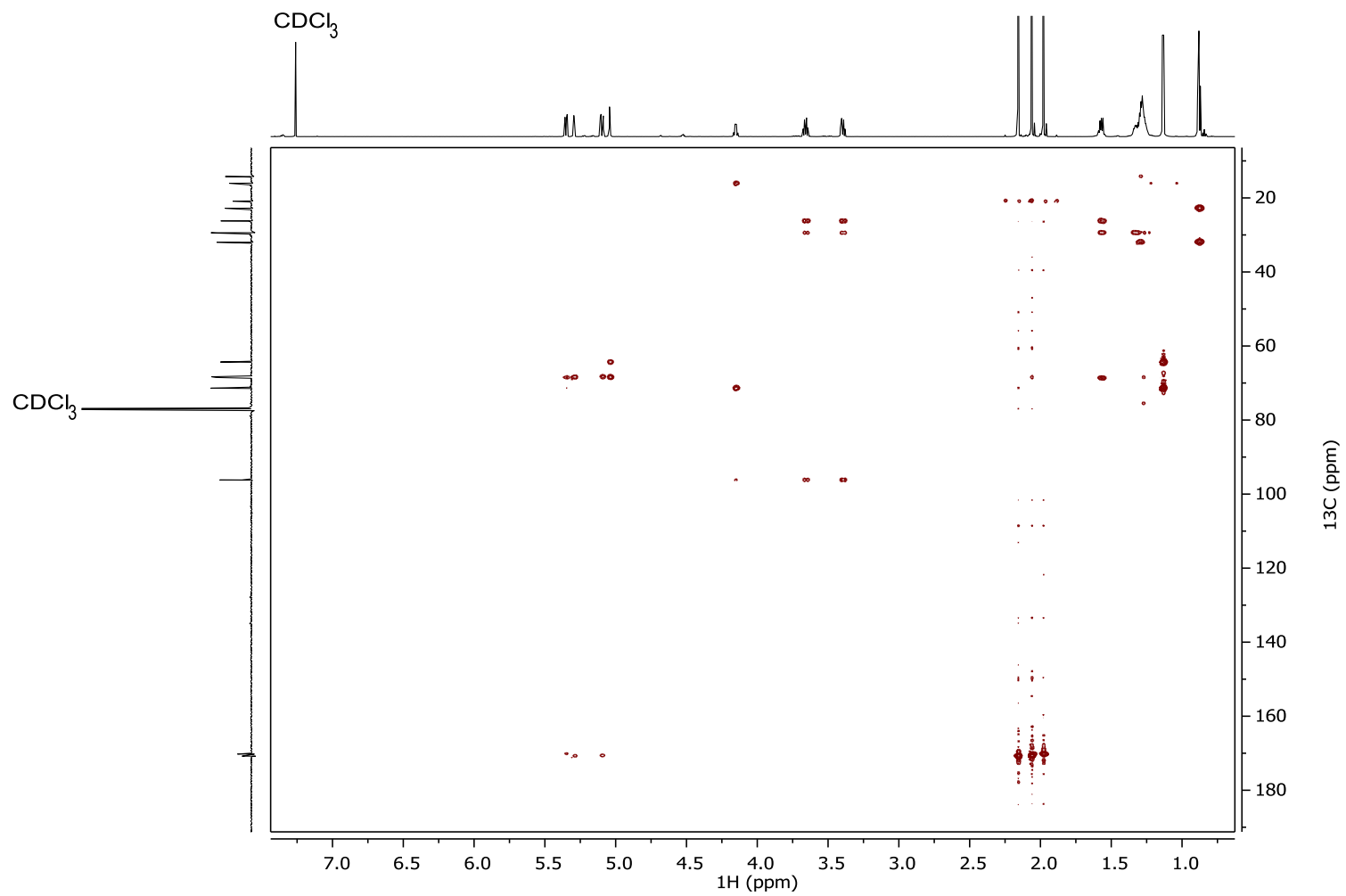
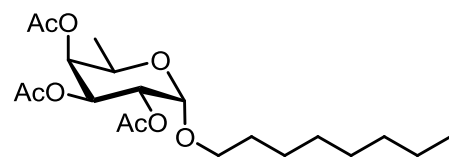
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-fucopyranoside



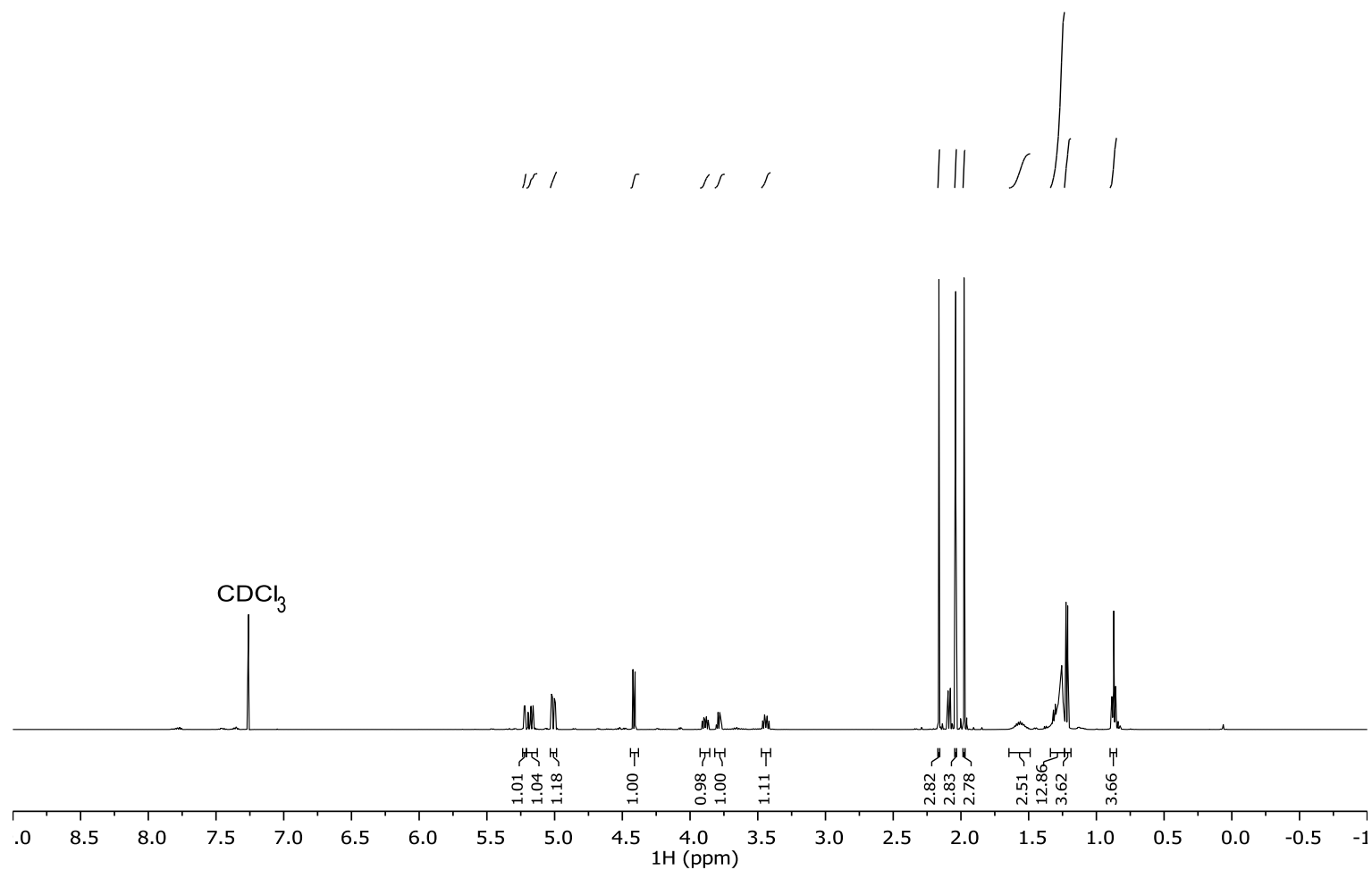
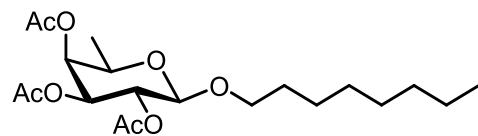
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-fucopyranoside



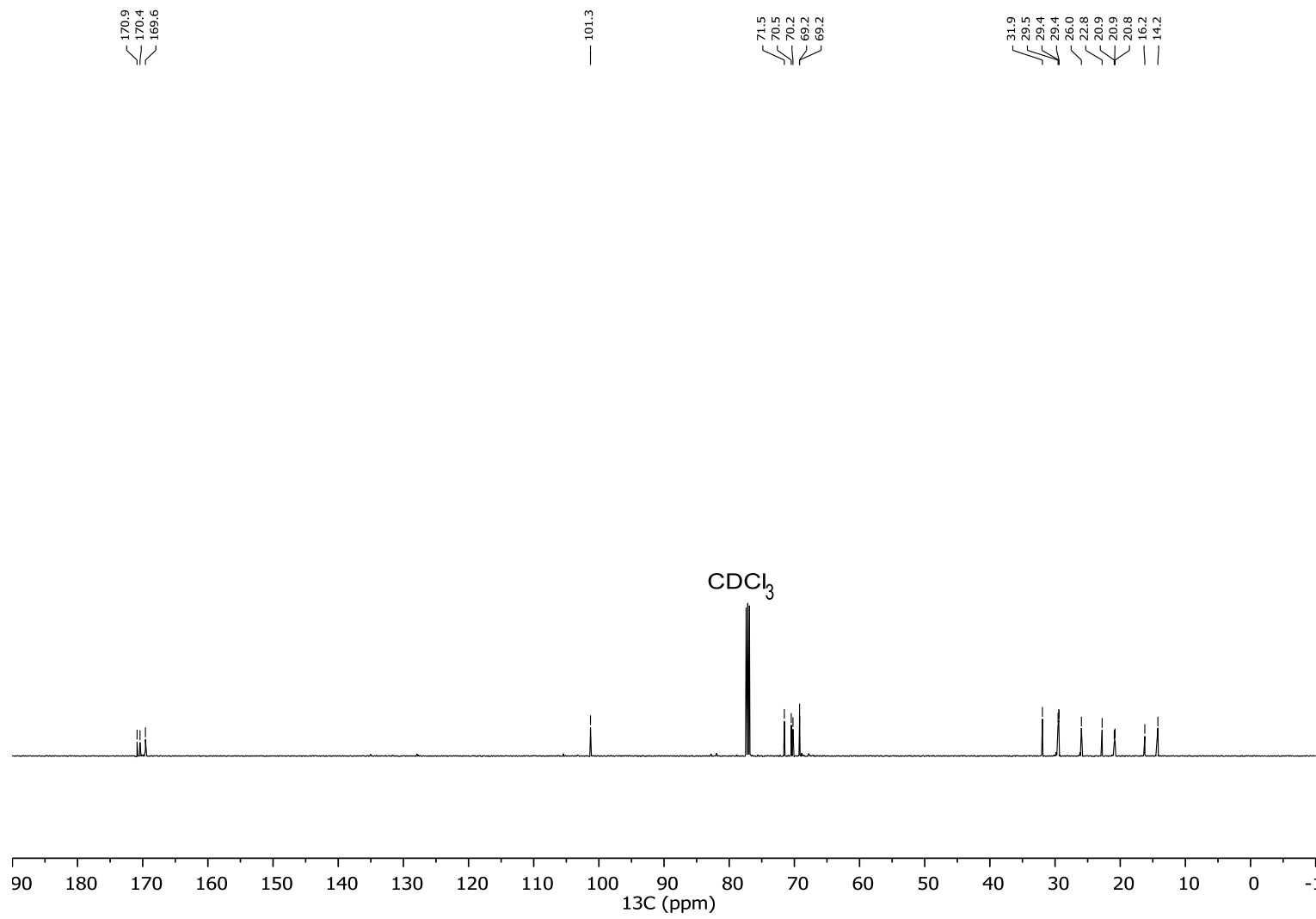
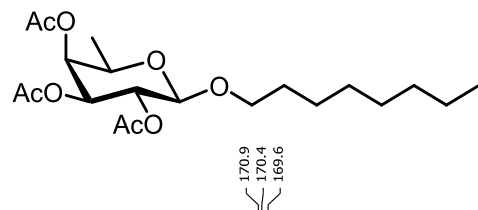
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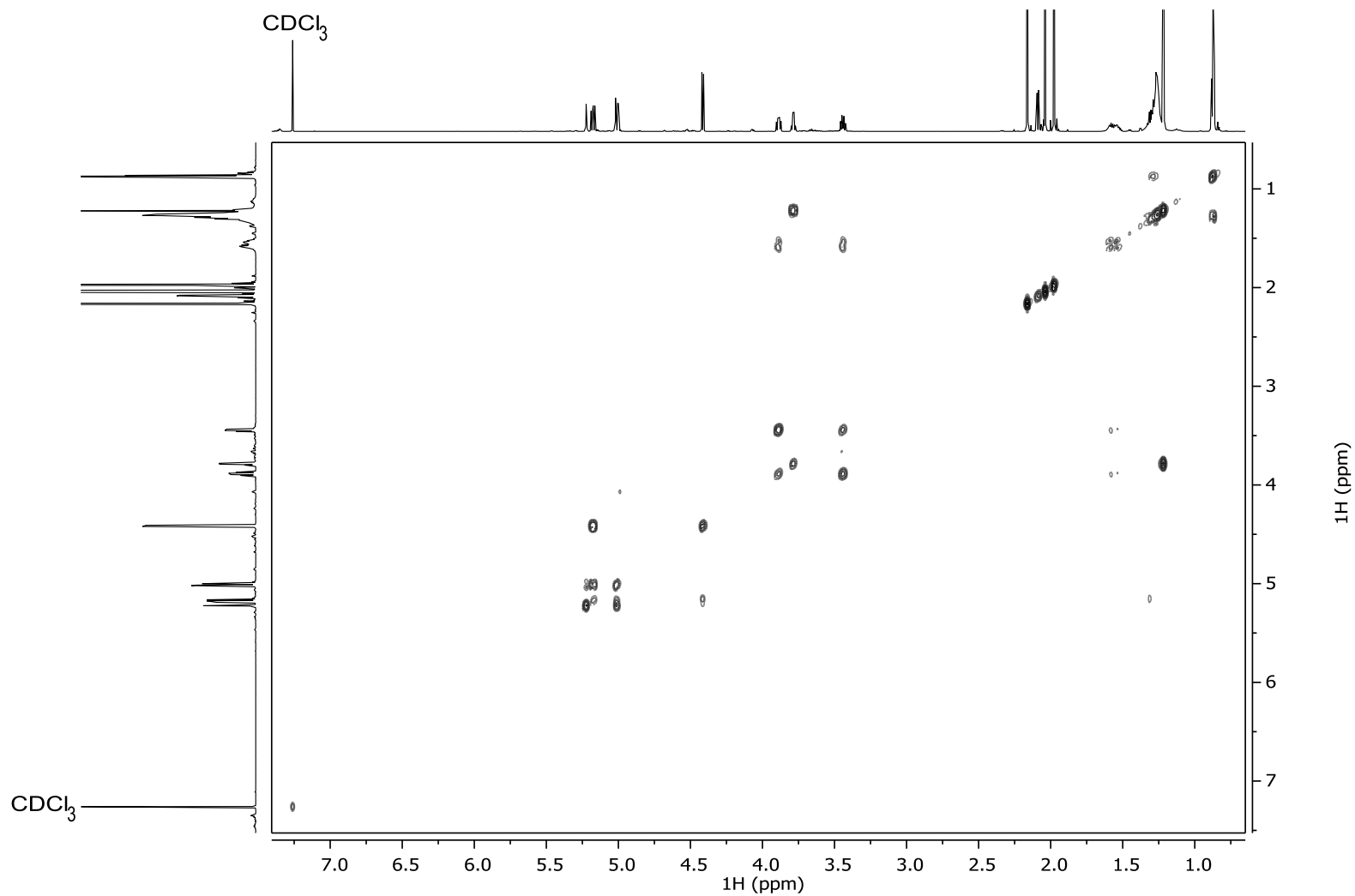
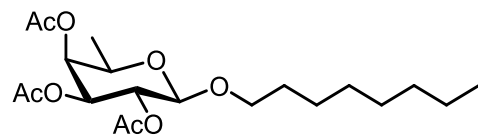
¹H NMR (500 MHz, CDCl₃) *n*-octyl 2,3,4-tri-*O*-acetyl-β-*D*-fucopyranoside



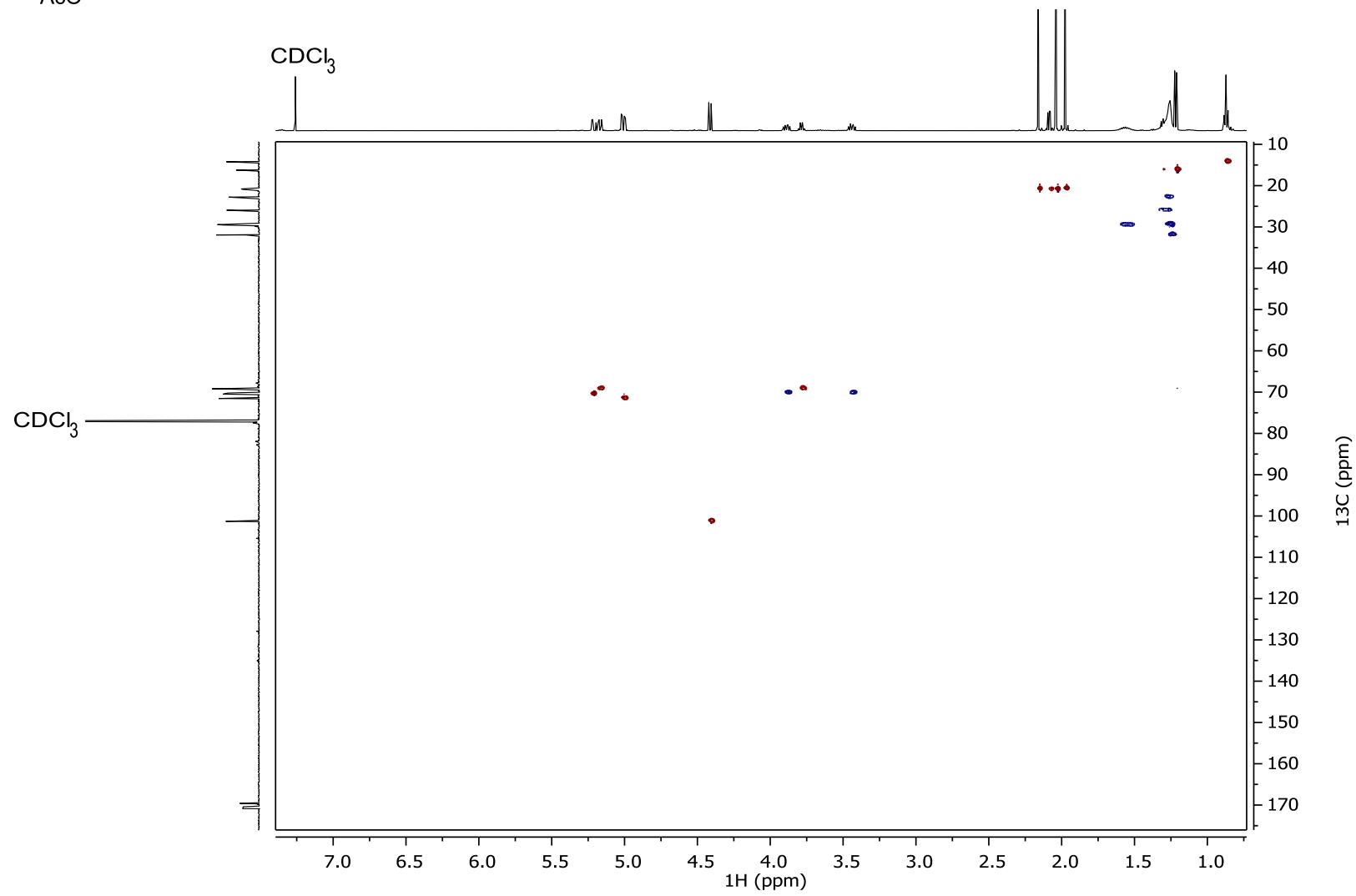
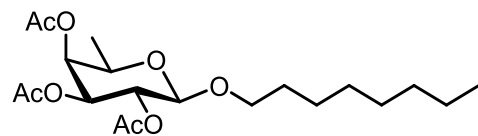
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-fucopyranoside



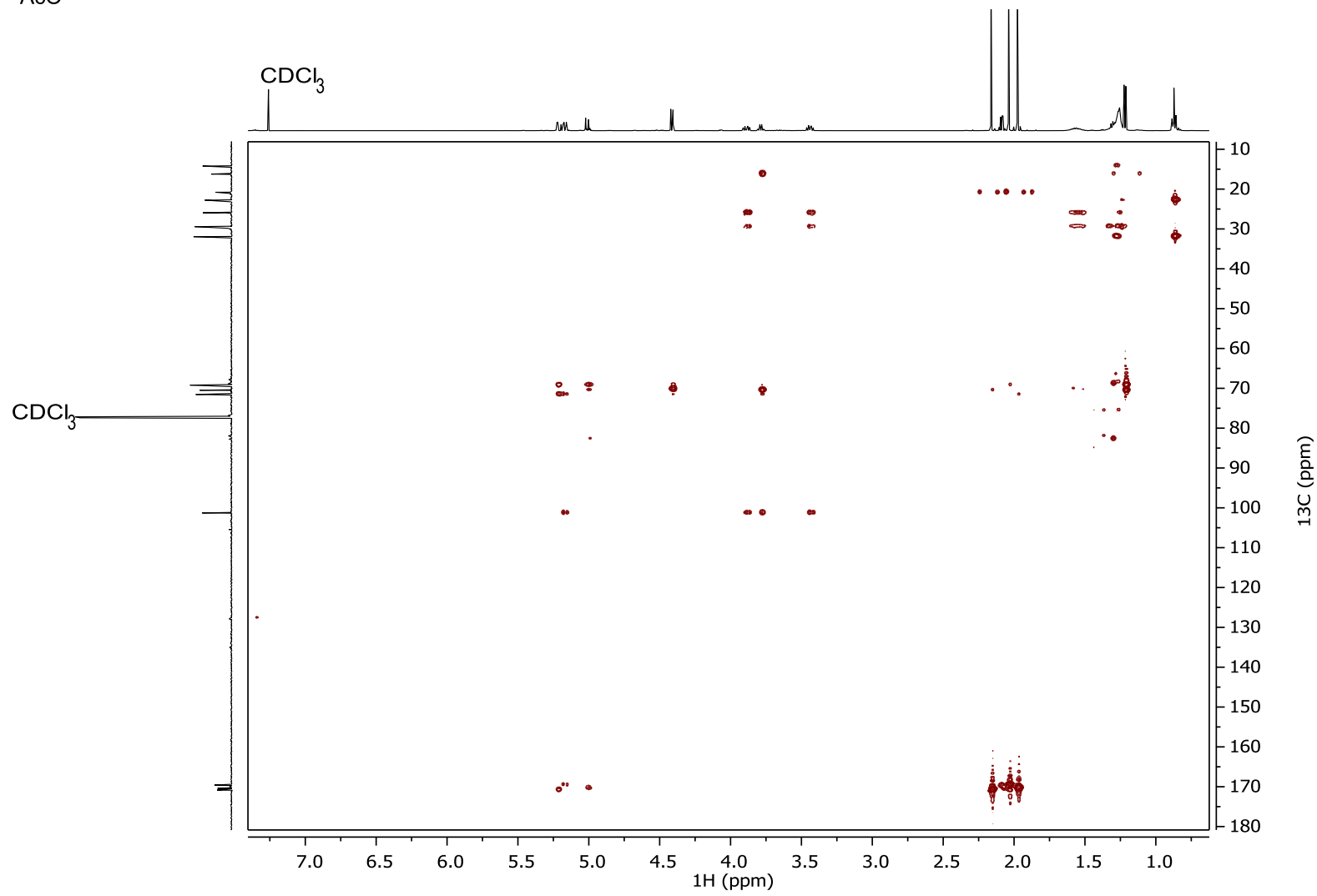
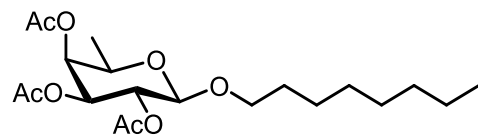
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-fucopyranoside



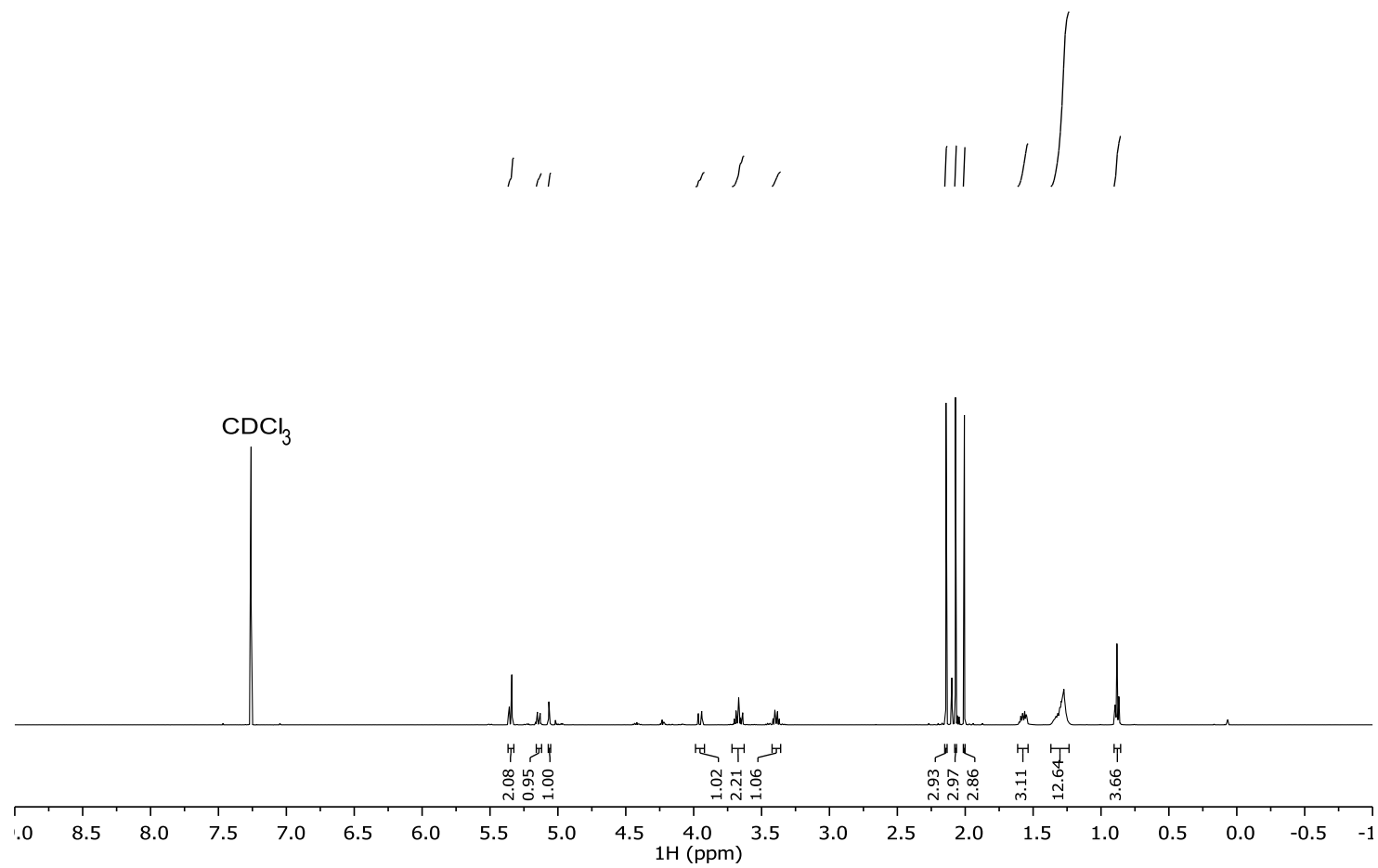
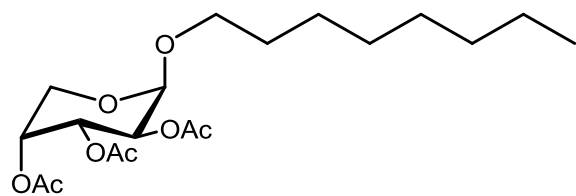
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-fucopyranoside



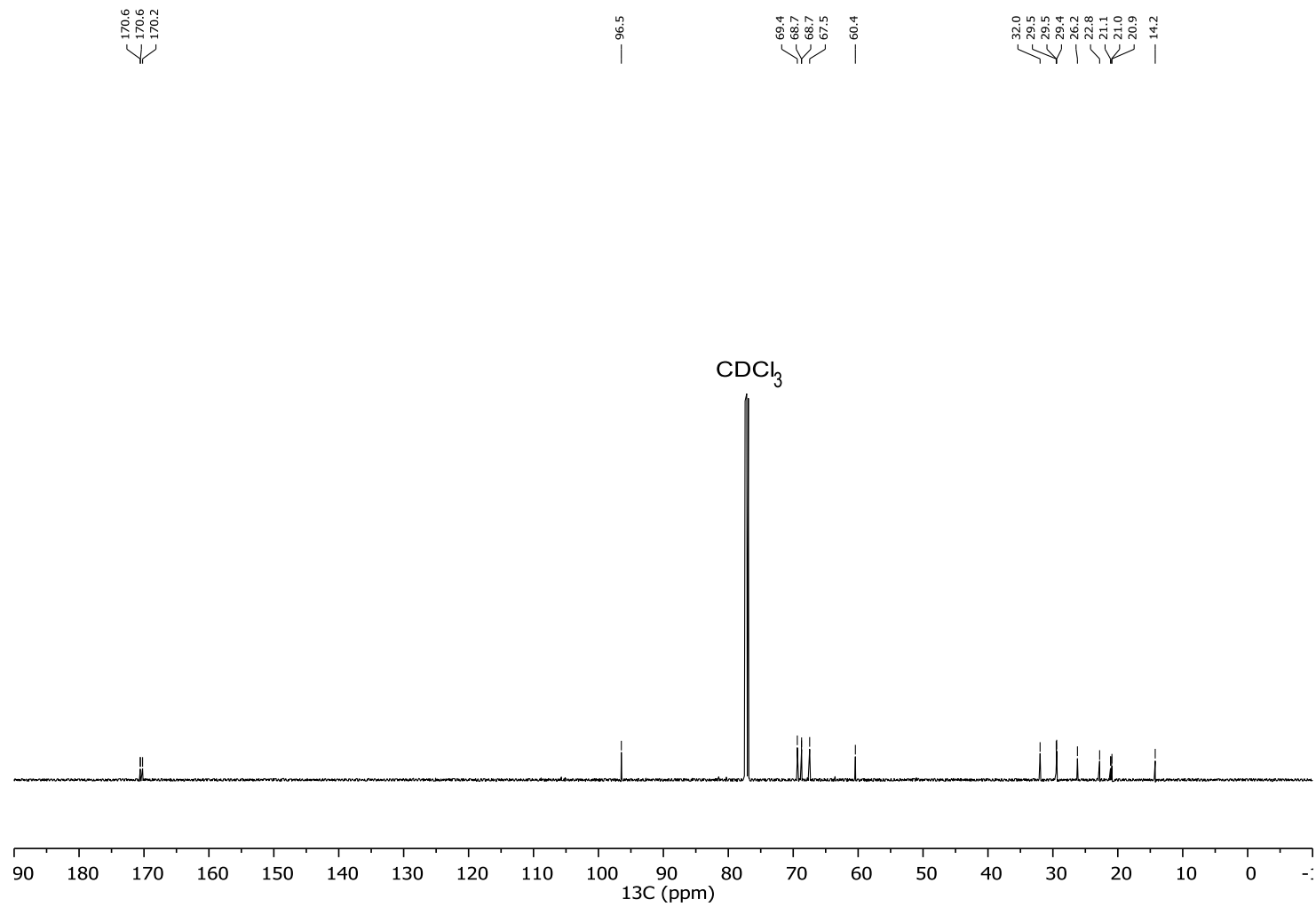
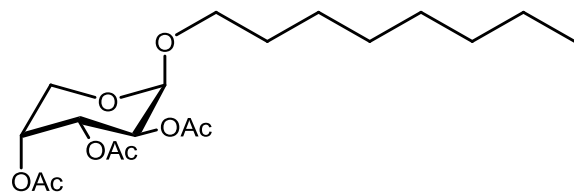
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-fucopyranoside



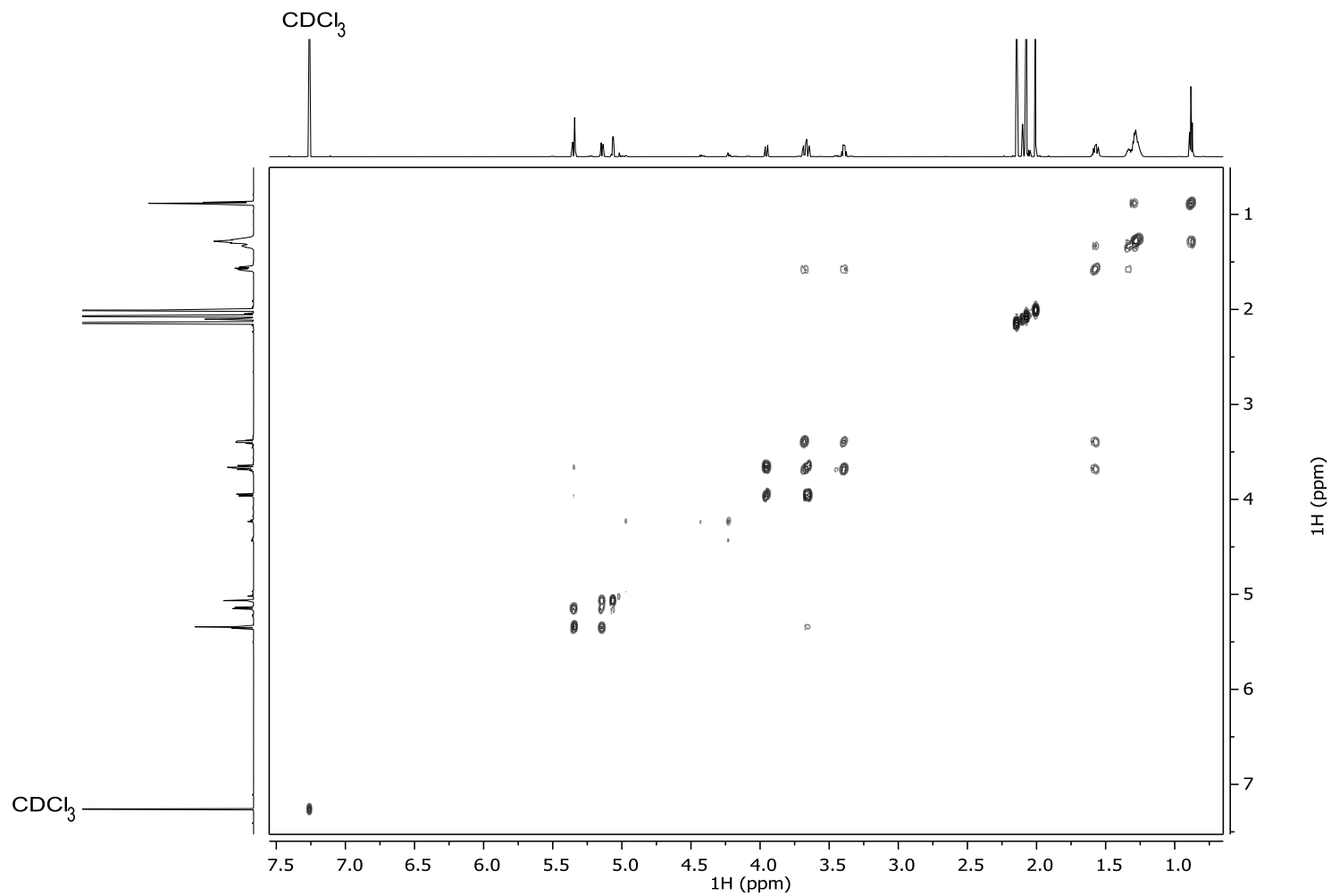
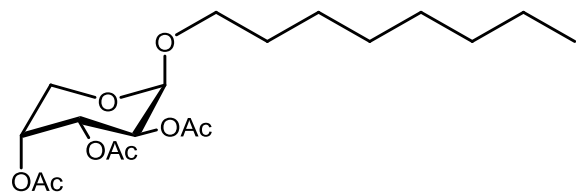
^1H NMR (500 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-arabinopyranoside



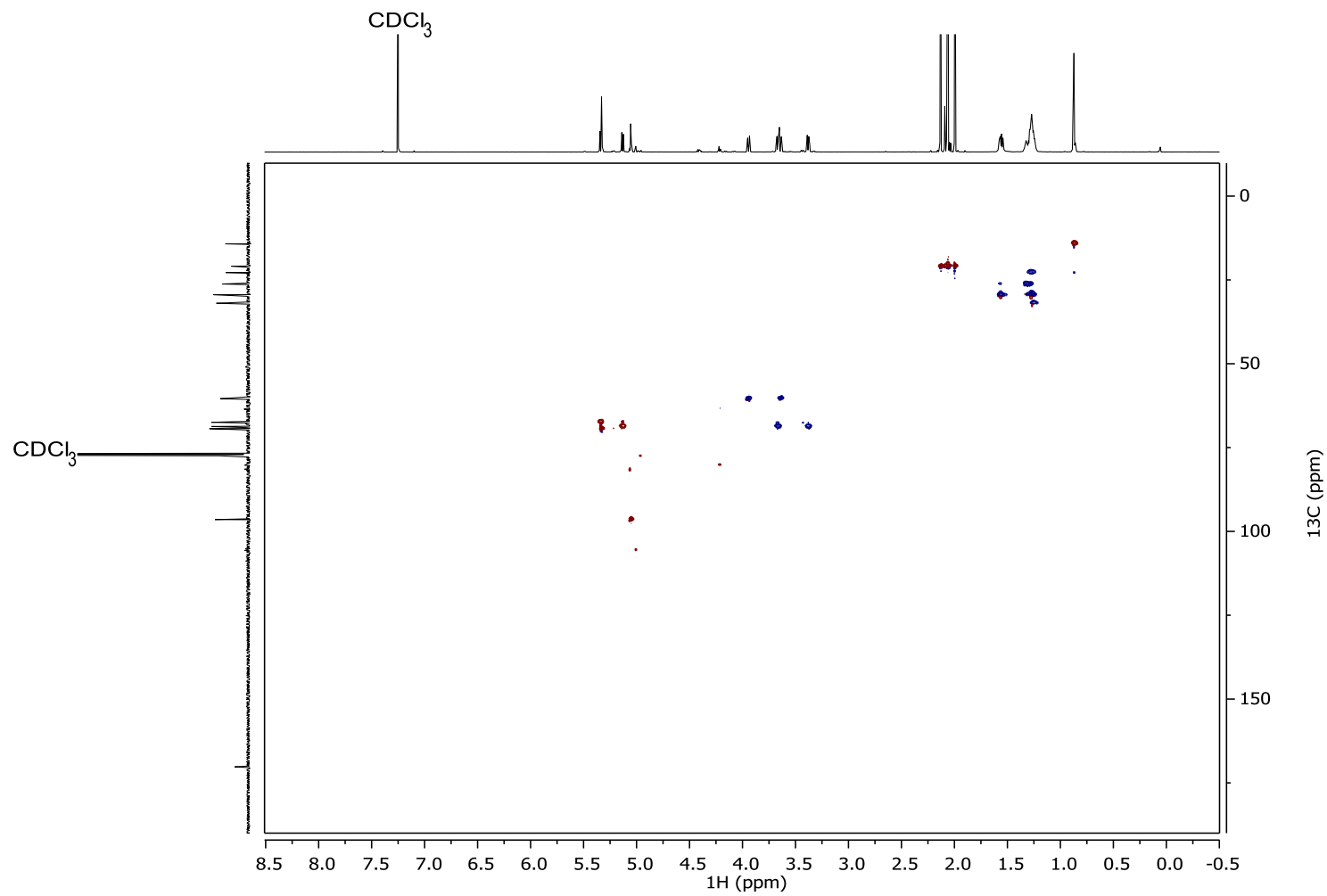
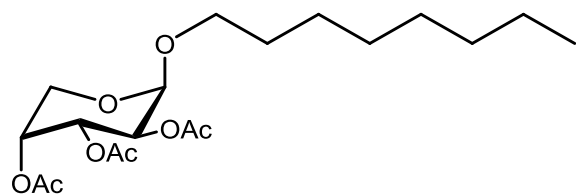
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-arabinopyranoside



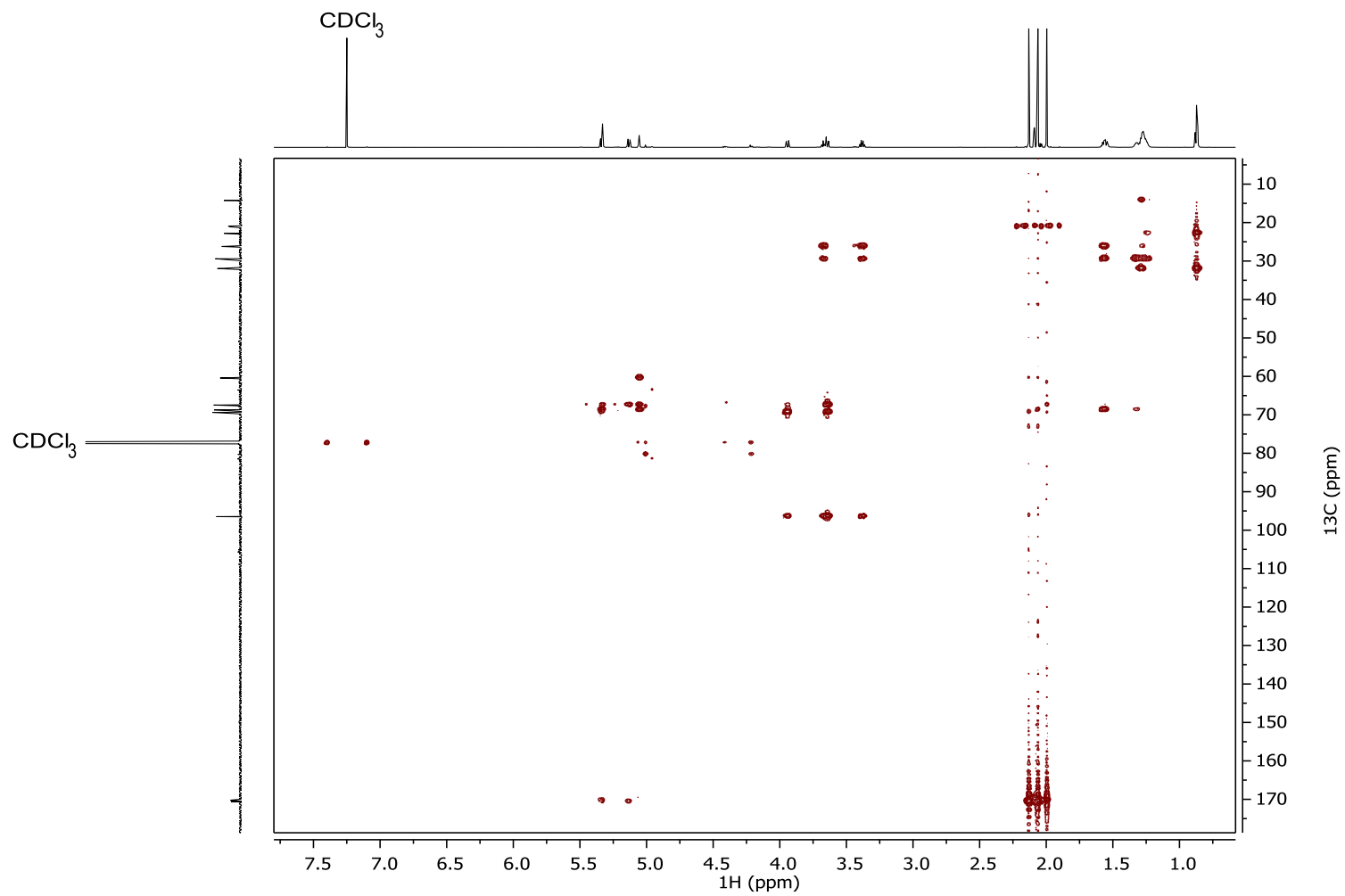
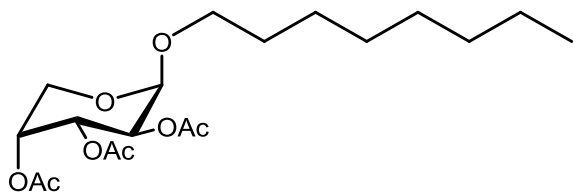
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-arabinopyranoside



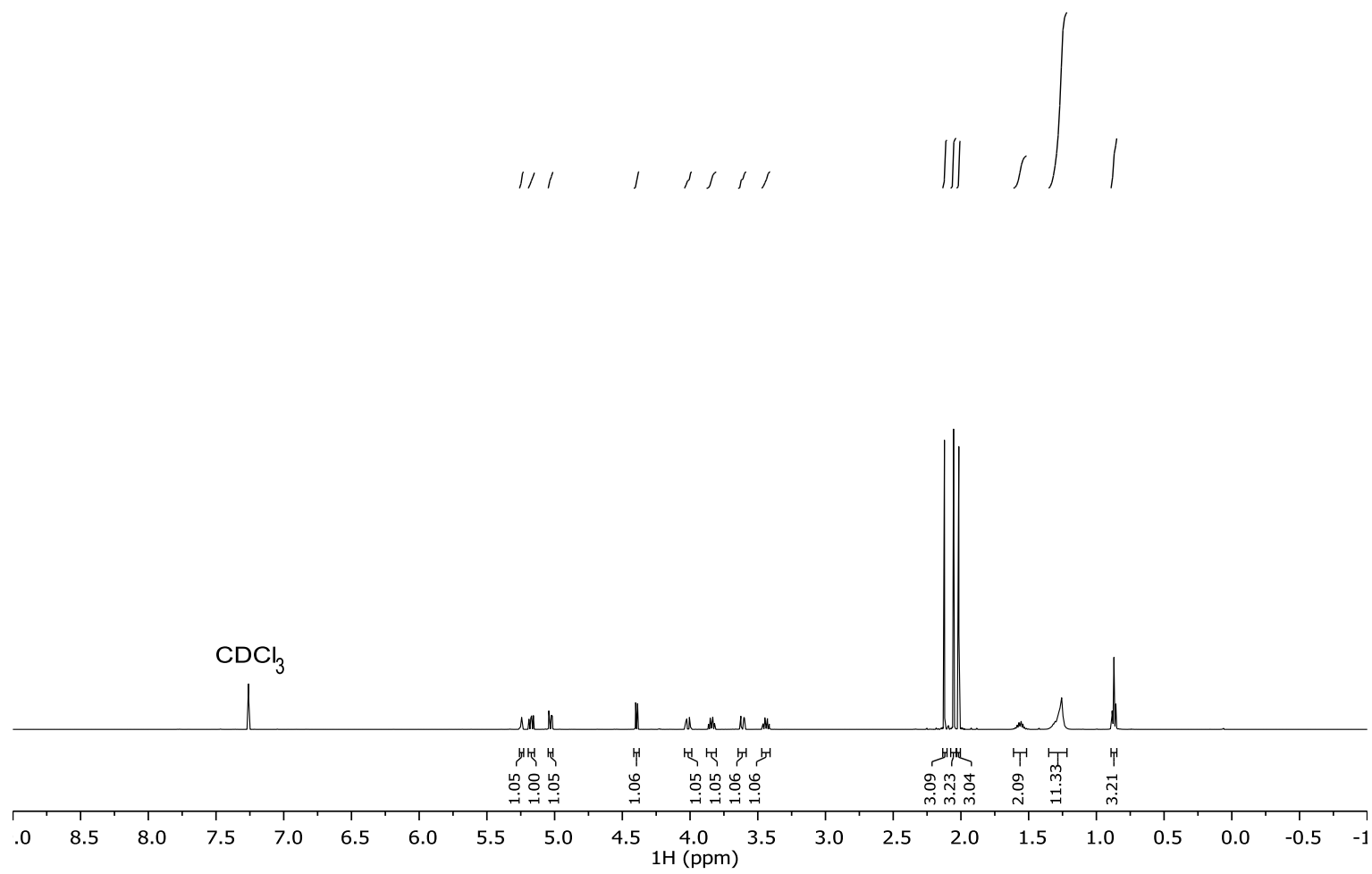
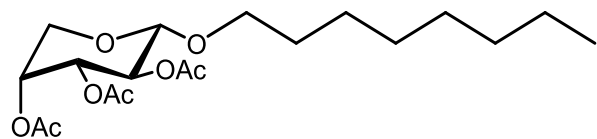
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-arabinopyranoside



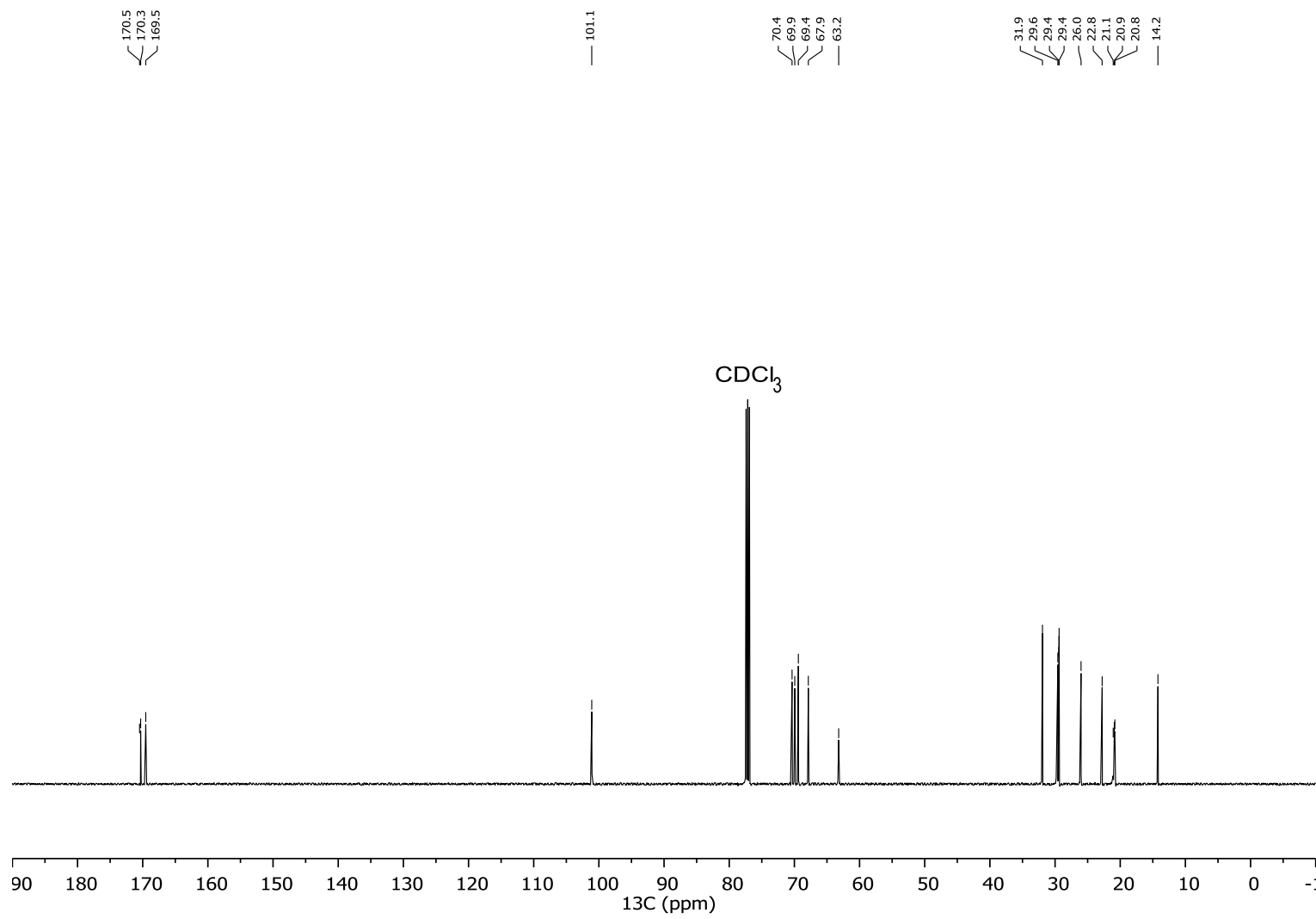
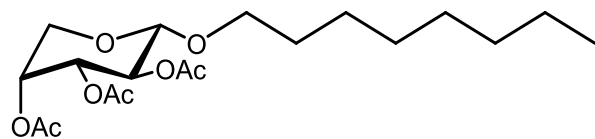
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-arabinopyranoside



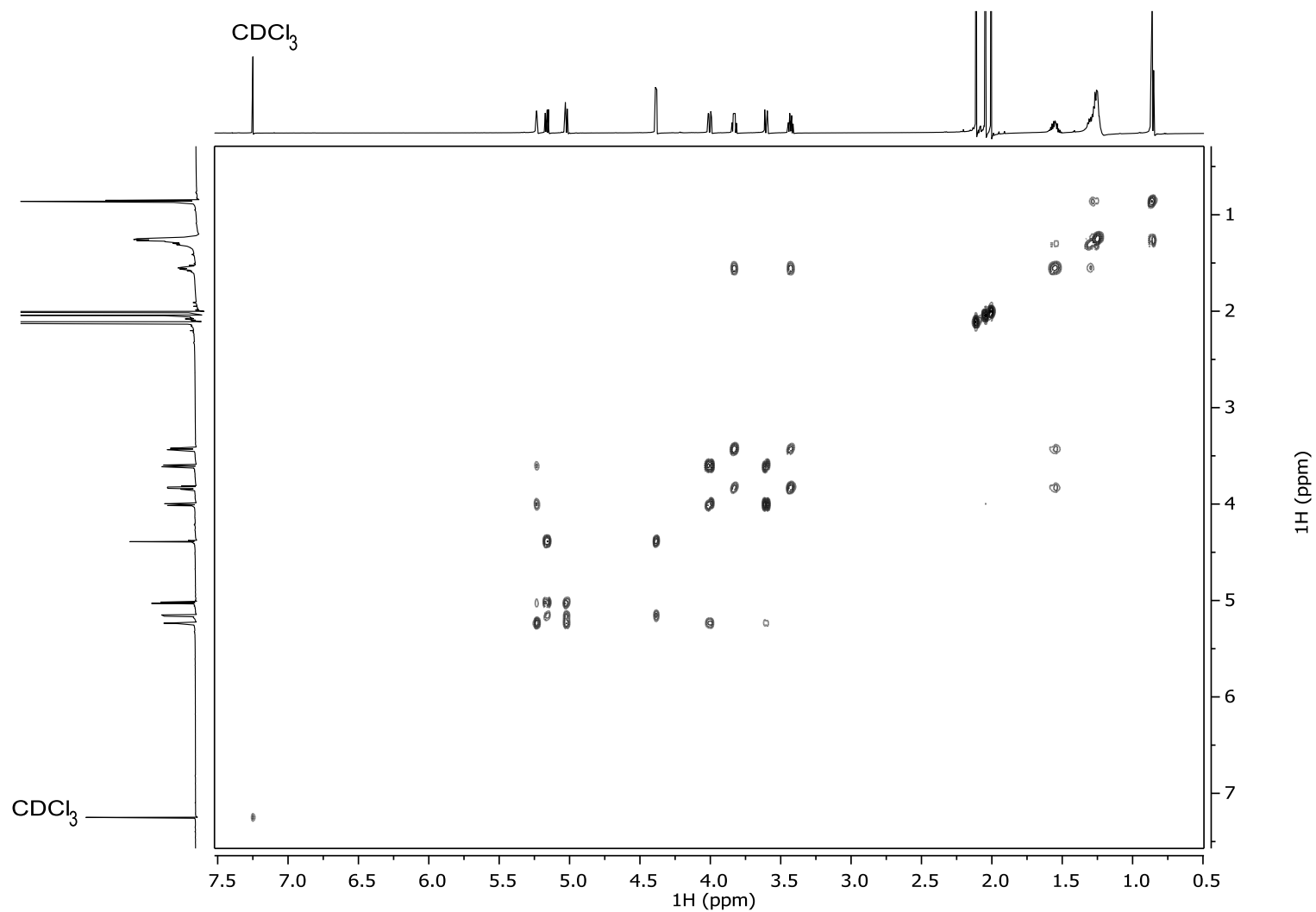
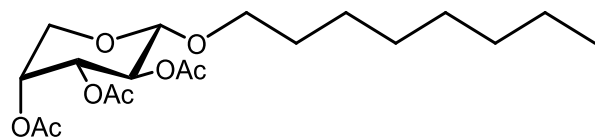
^1H NMR (500 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-arabinopyranoside



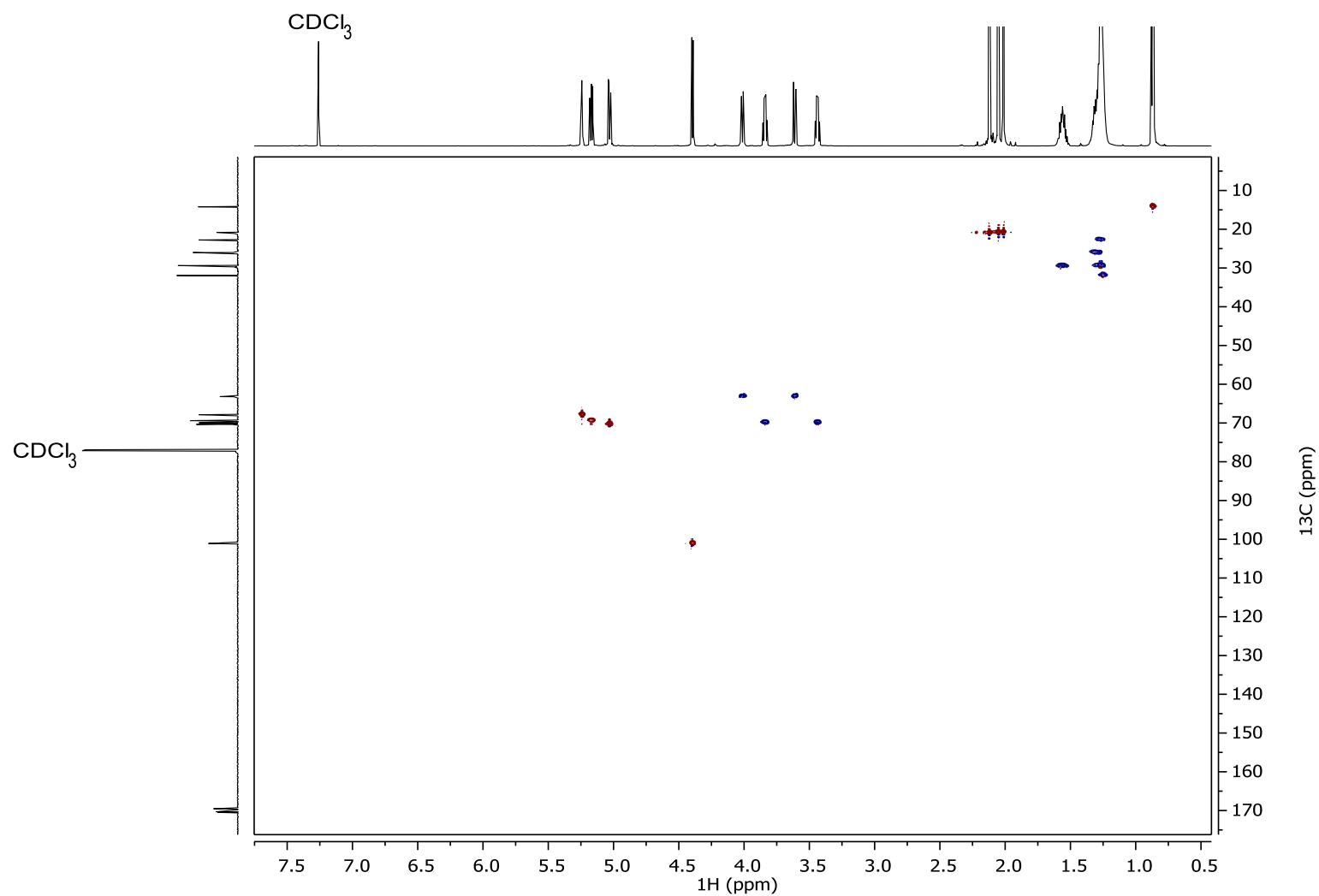
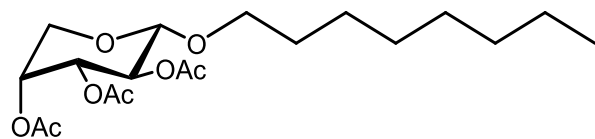
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-arabinopyranoside



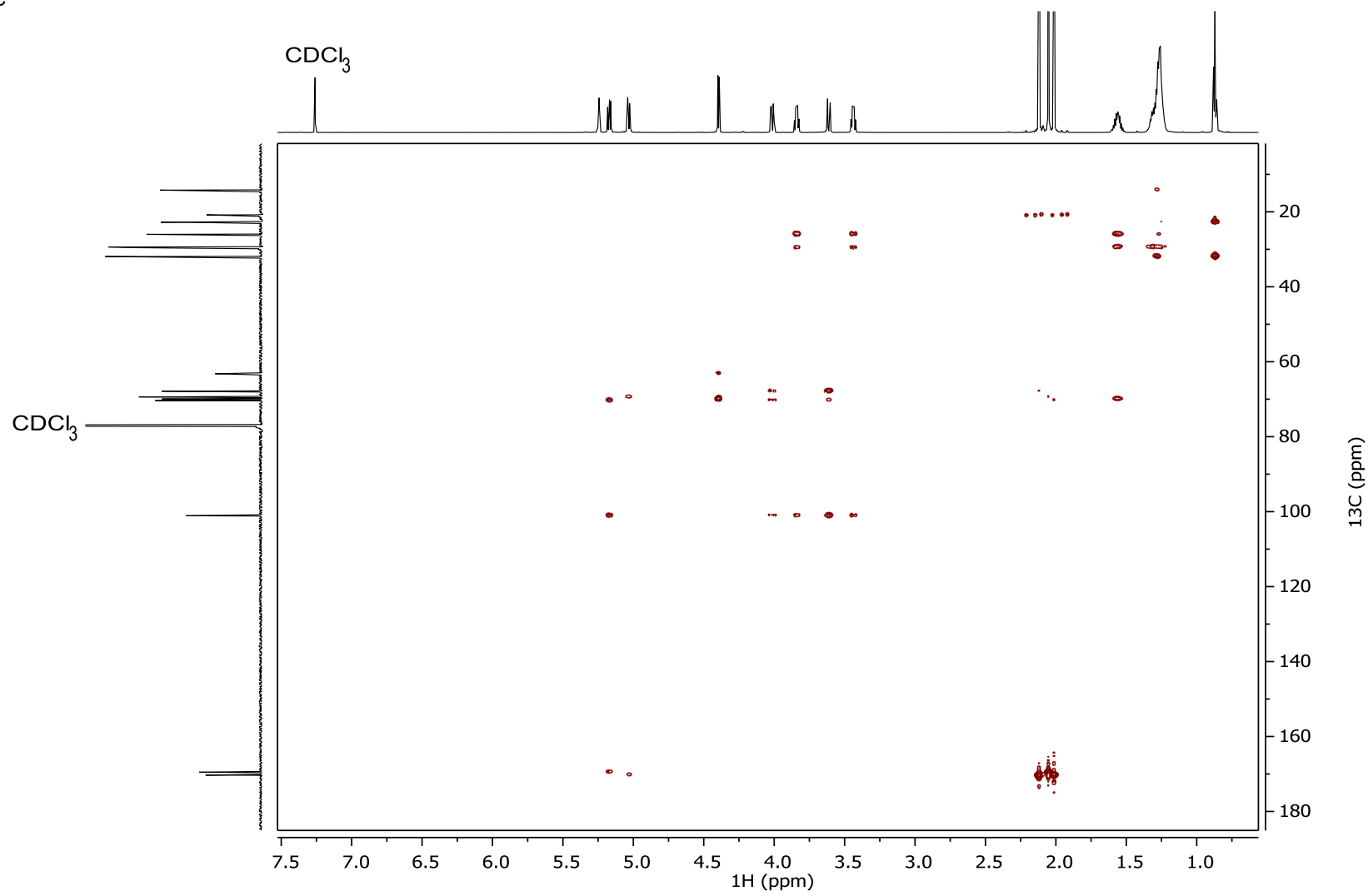
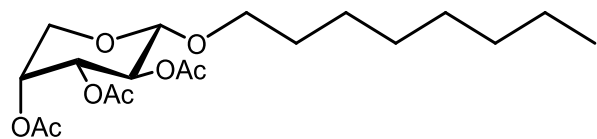
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-arabinopyranoside



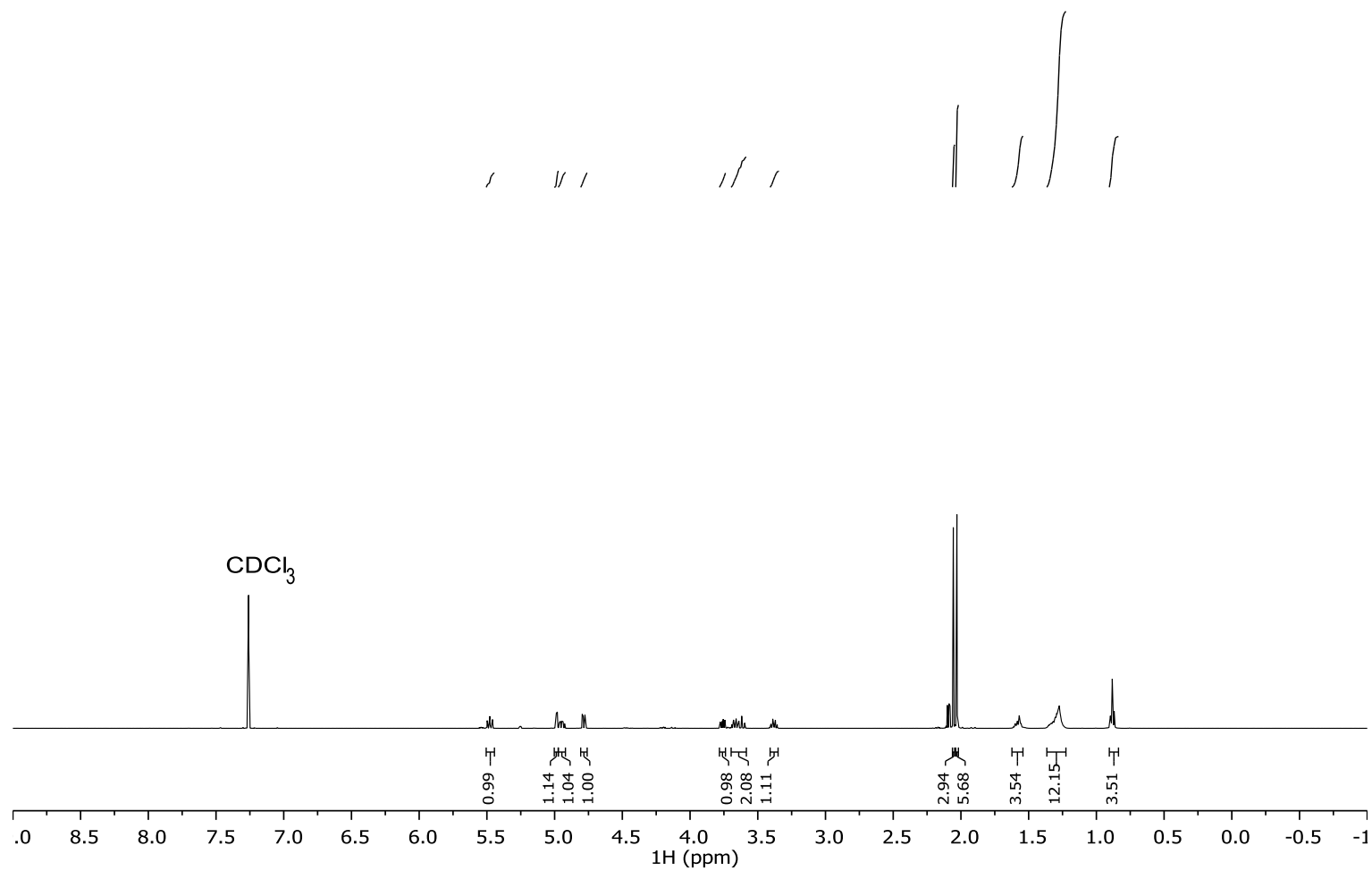
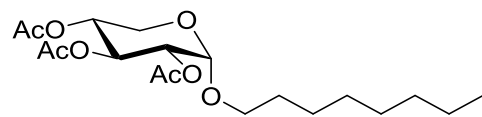
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-arabinopyranoside



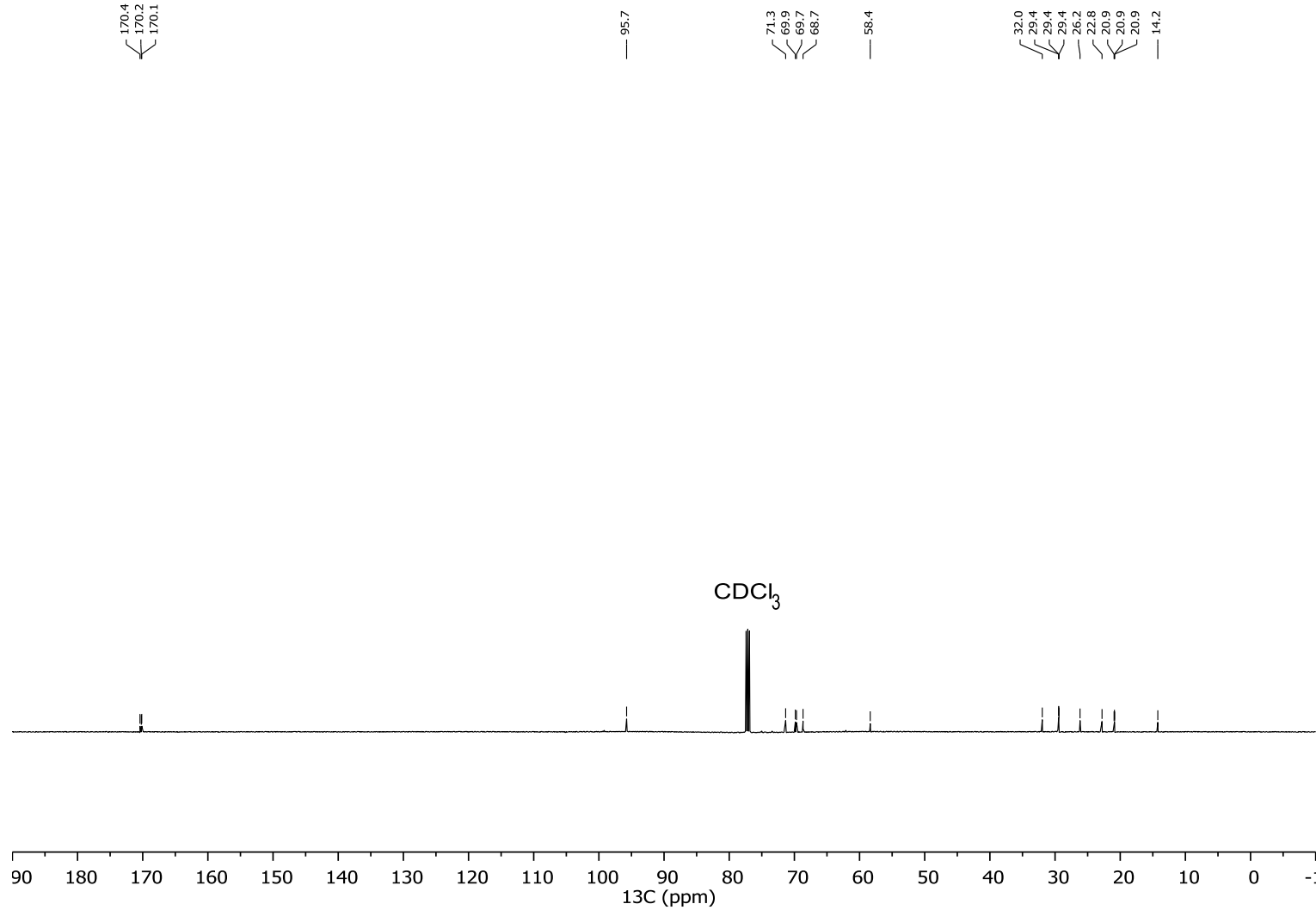
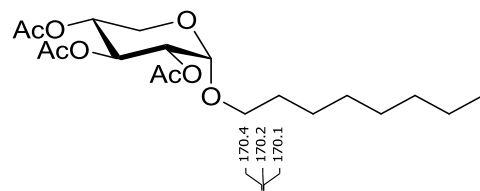
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-arabinopyranoside



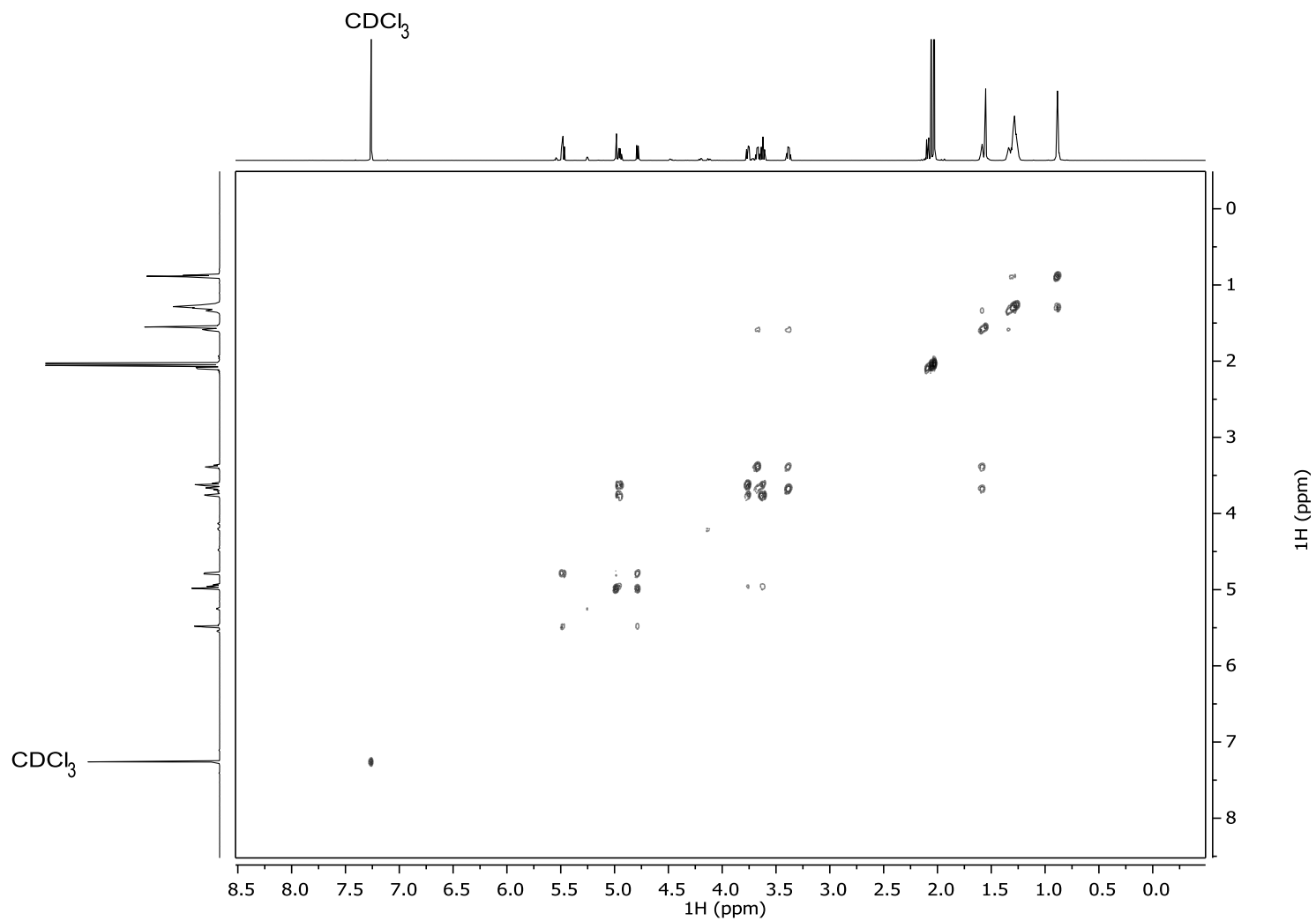
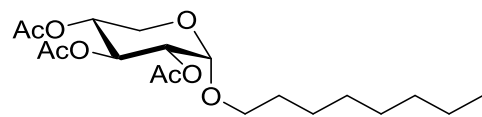
^1H NMR (500 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-xylopyranoside



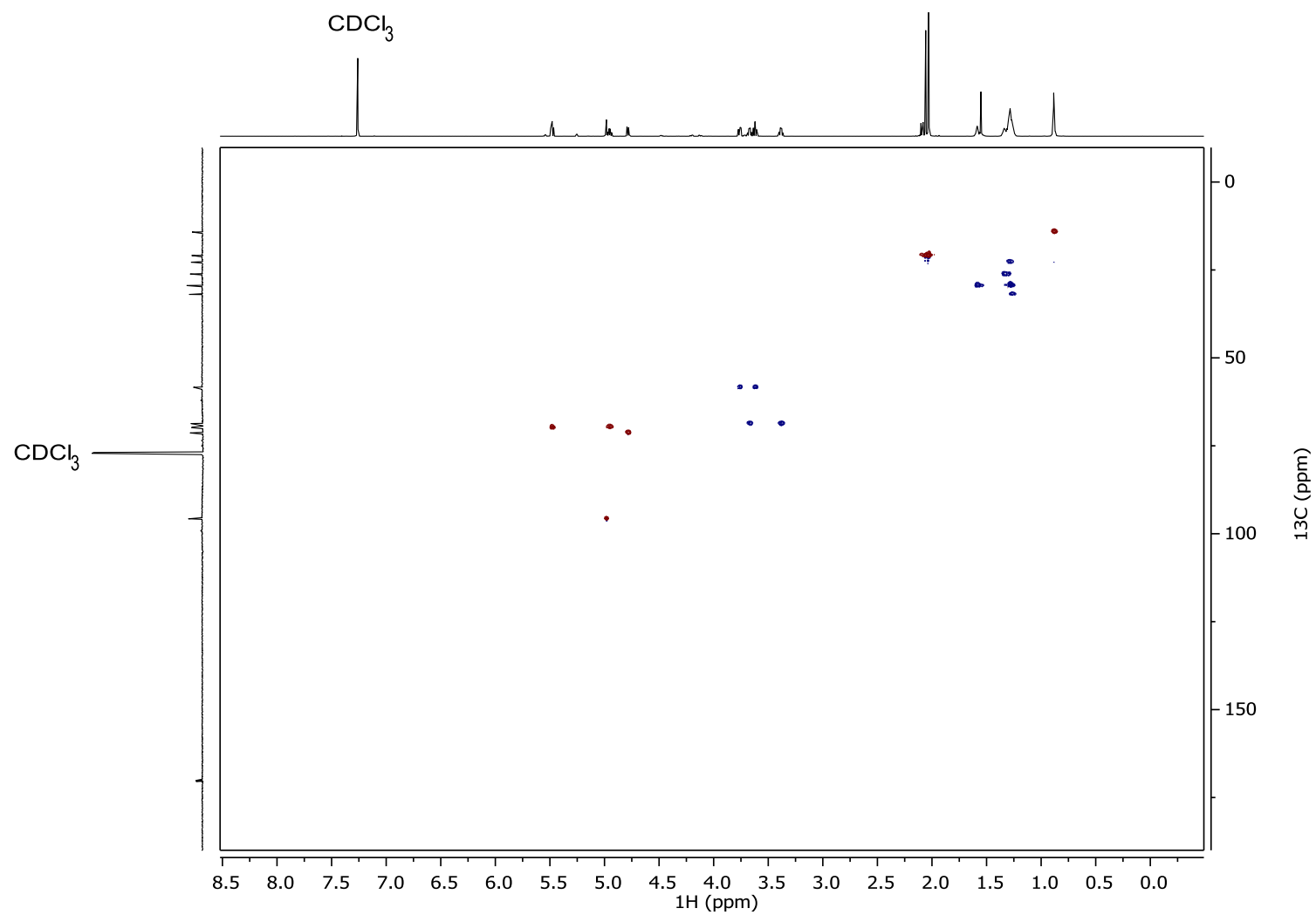
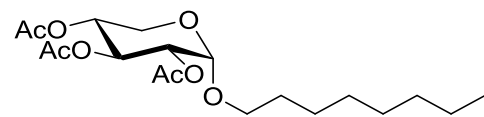
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-xylopyranoside



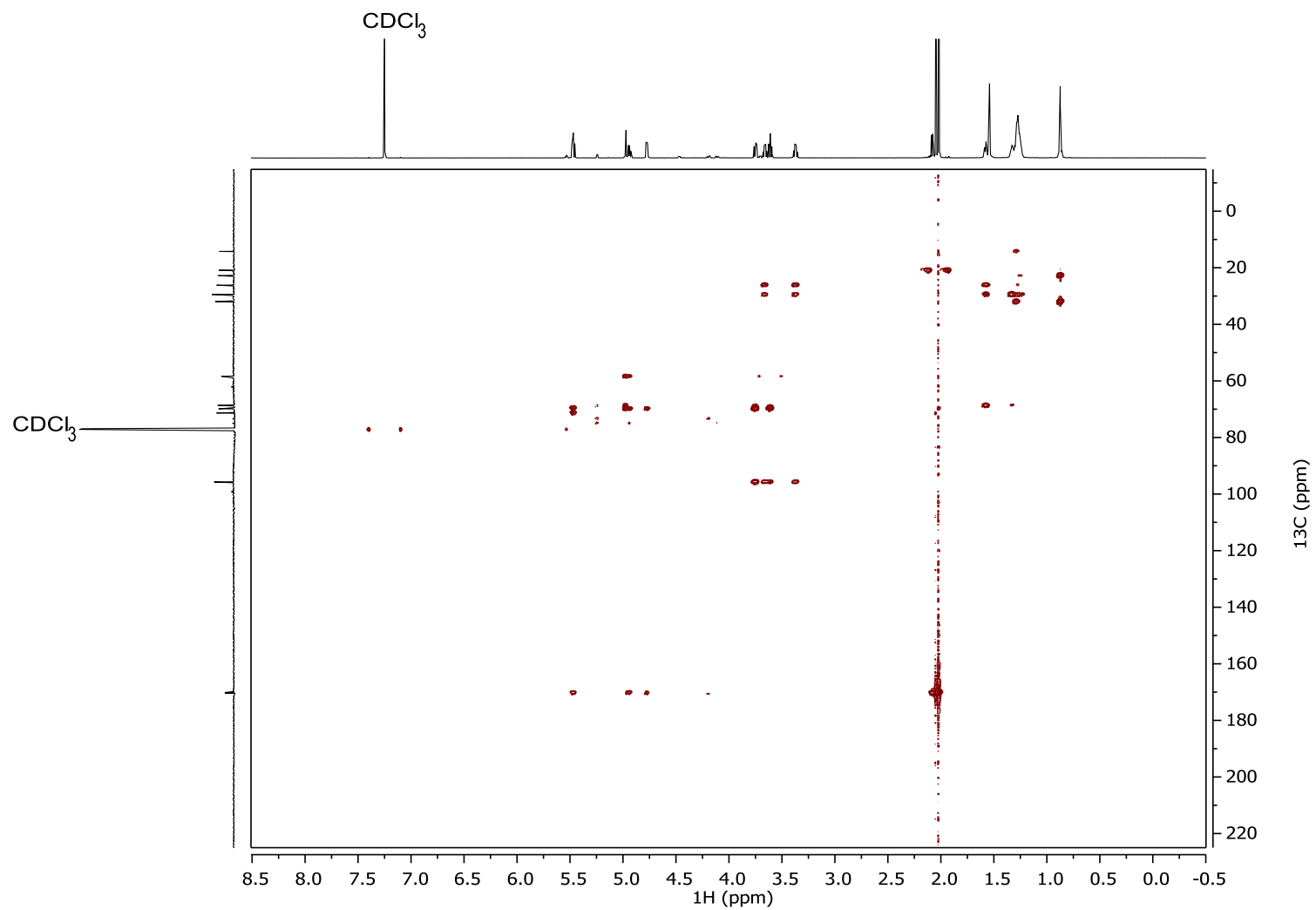
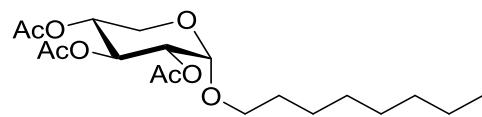
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-xylopyranoside



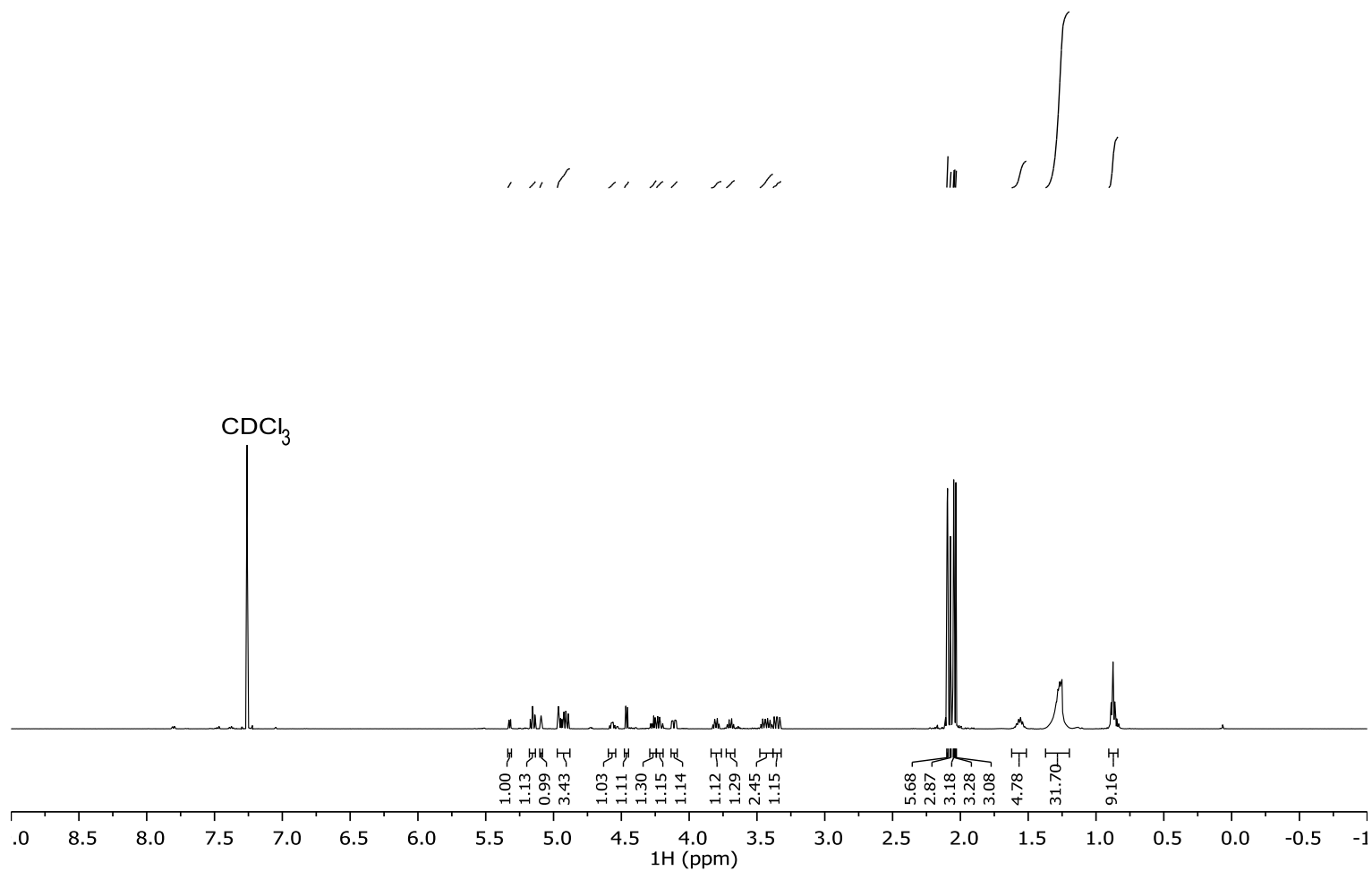
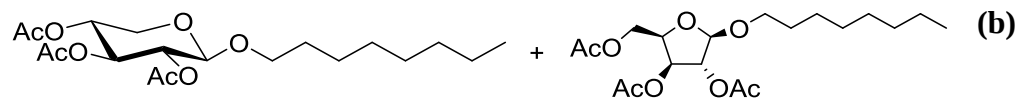
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-xylopyranoside



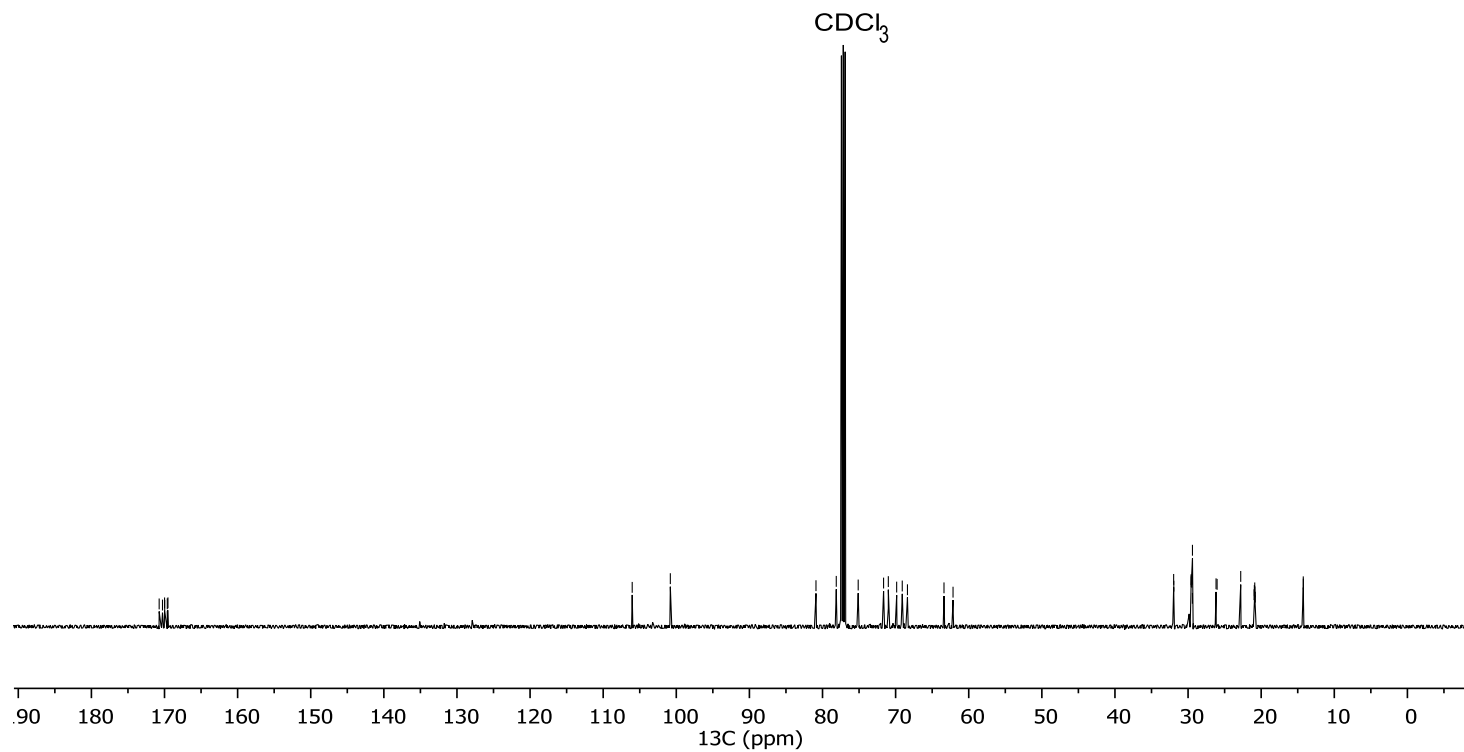
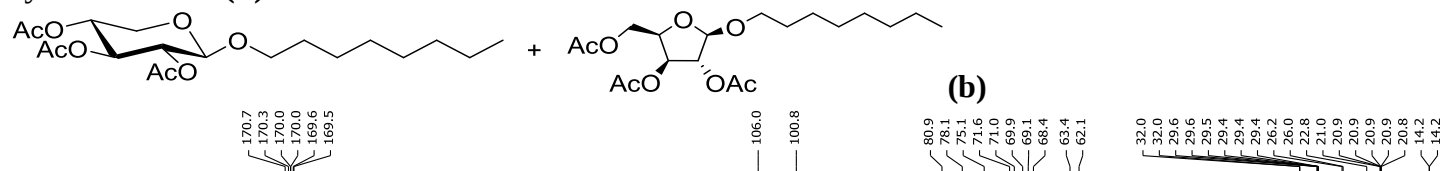
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,4-tri-*O*-acetyl- α -D-xylopyranoside



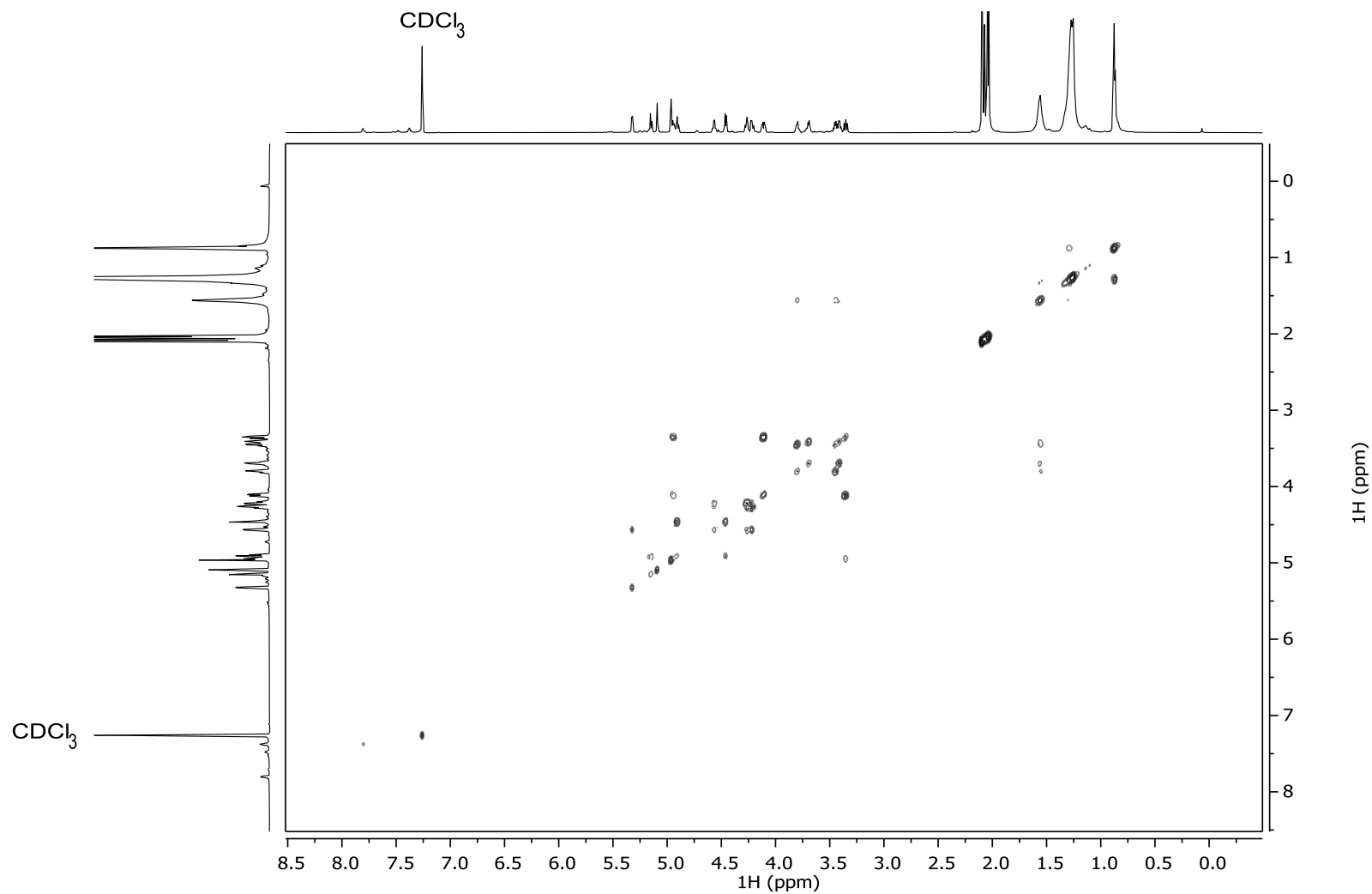
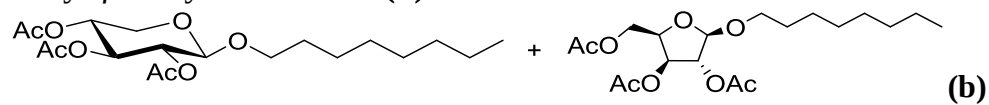
¹H NMR (500 MHz, CDCl₃) Mixture of *n*-octyl 2,3,4-tri-*O*-acetyl-β-D-xylopyranoside + *n*-octyl 2,3,5-tri-*O*-acetyl-β-D-xylofuranoside **(b)**



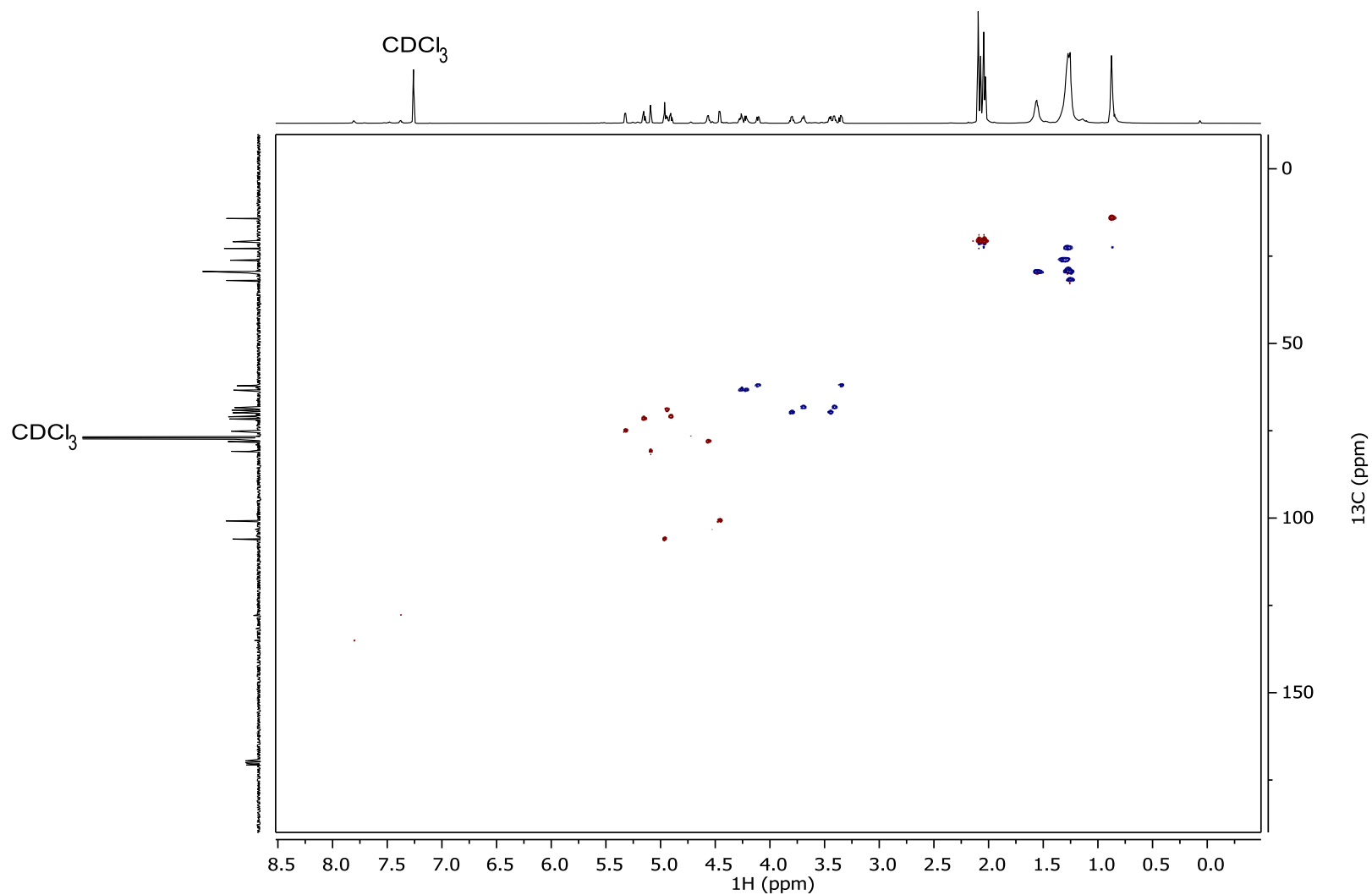
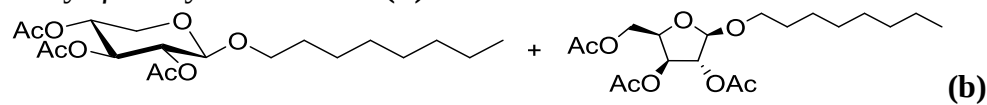
^{13}C NMR (126 MHz, CDCl_3) Mixture of *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-xylopyranoside + *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-xylofuranoside **(b)**



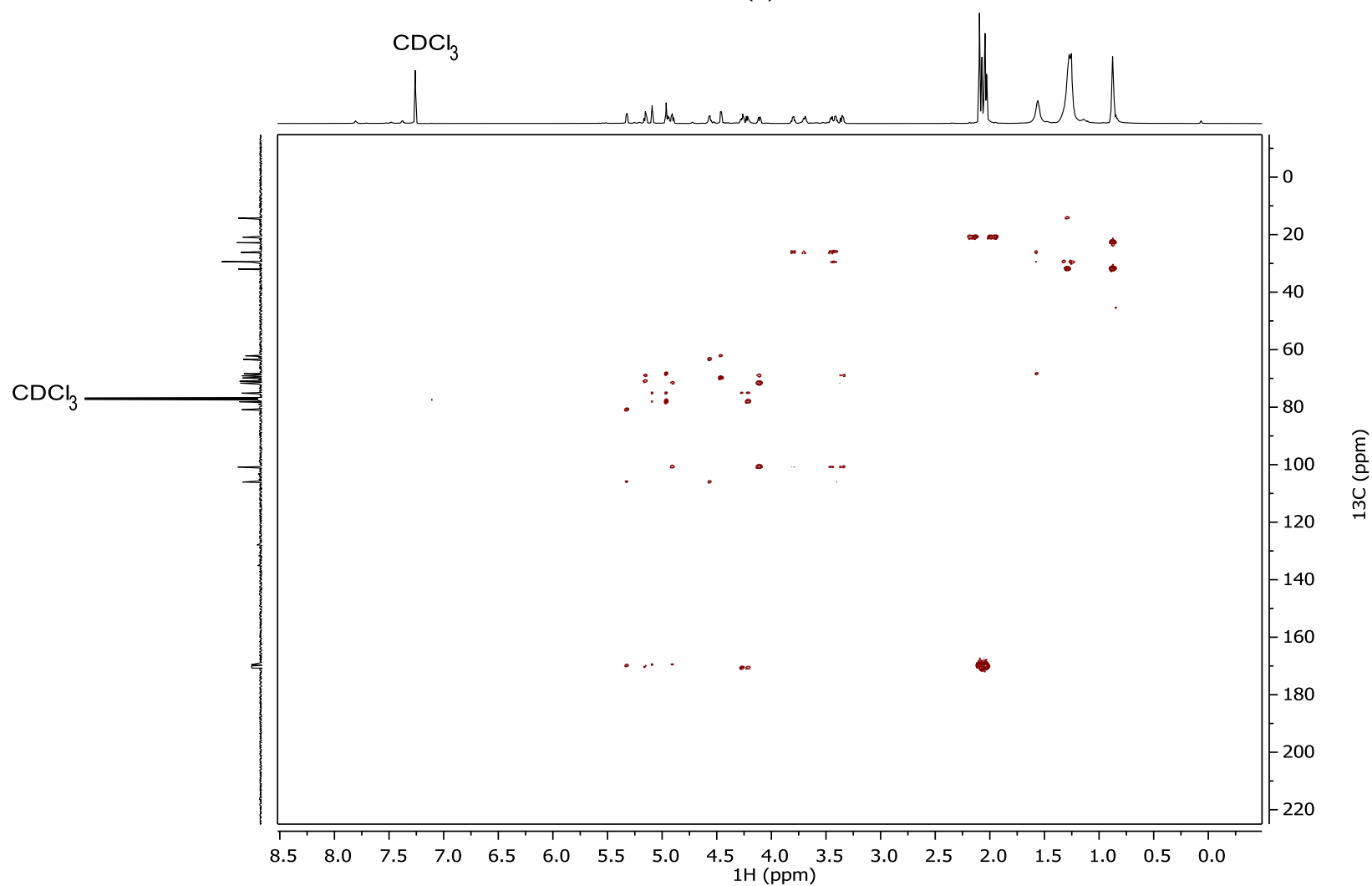
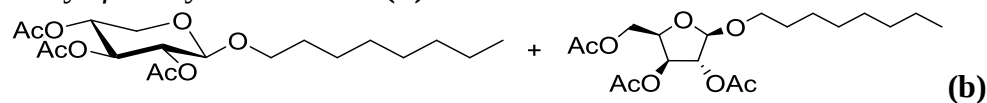
^1H - ^1H COSY NMR (126 MHz, CDCl_3) Mixture of *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-xylopyranoside + *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-xylofuranoside **(b)**



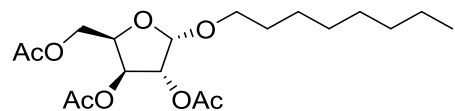
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) Mixture of *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-xylopyranoside + *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-xylofuranoside (b)



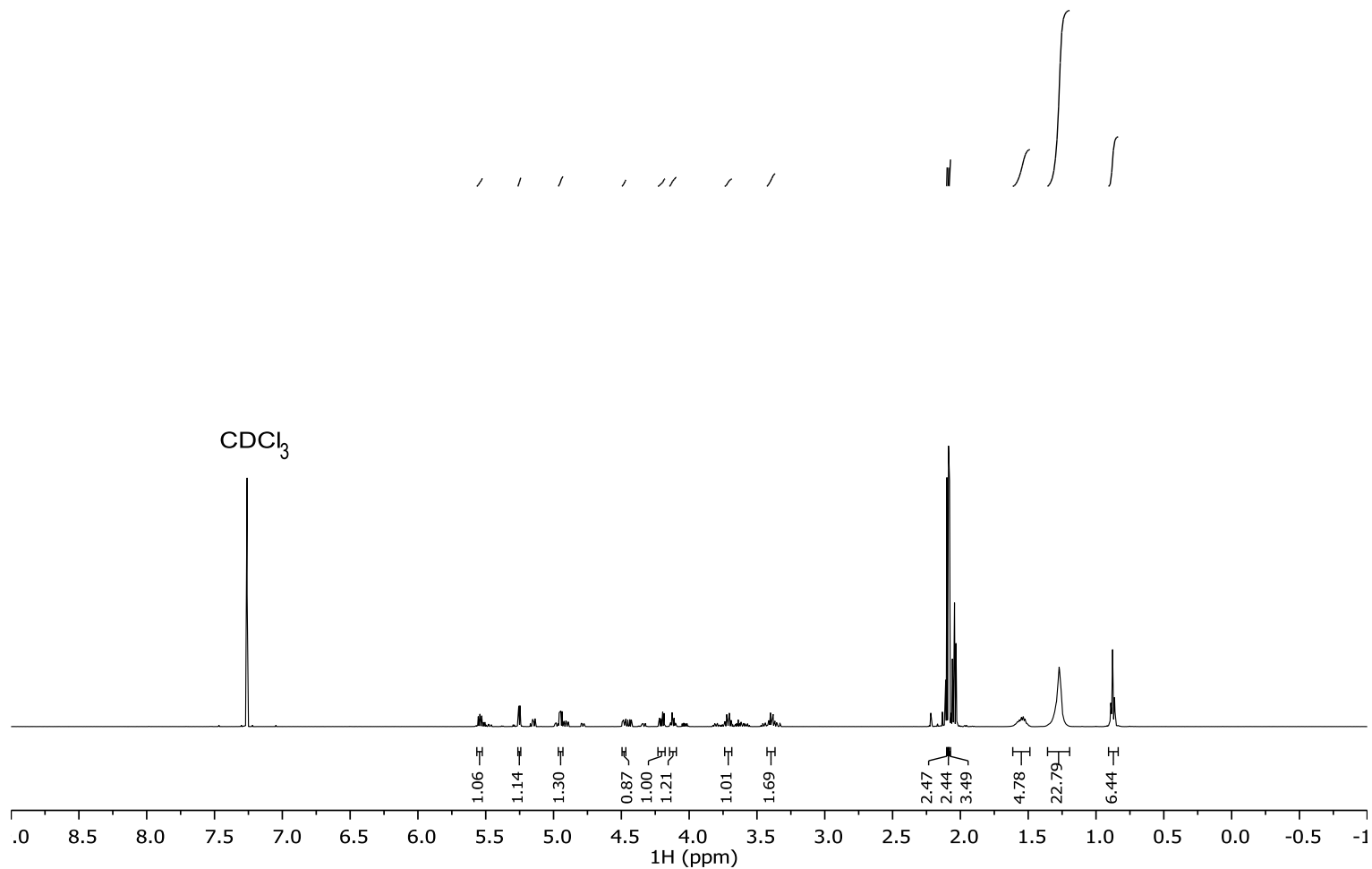
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) Mixture of *n*-octyl 2,3,4-tri-*O*-acetyl- β -D-xylopyranoside + *n*-octyl 2,3,5-tri-*O*-acetyl- β -D-xylofuranoside (b)



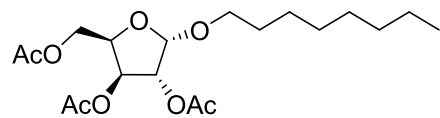
^1H NMR (500 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-xylofuranoside



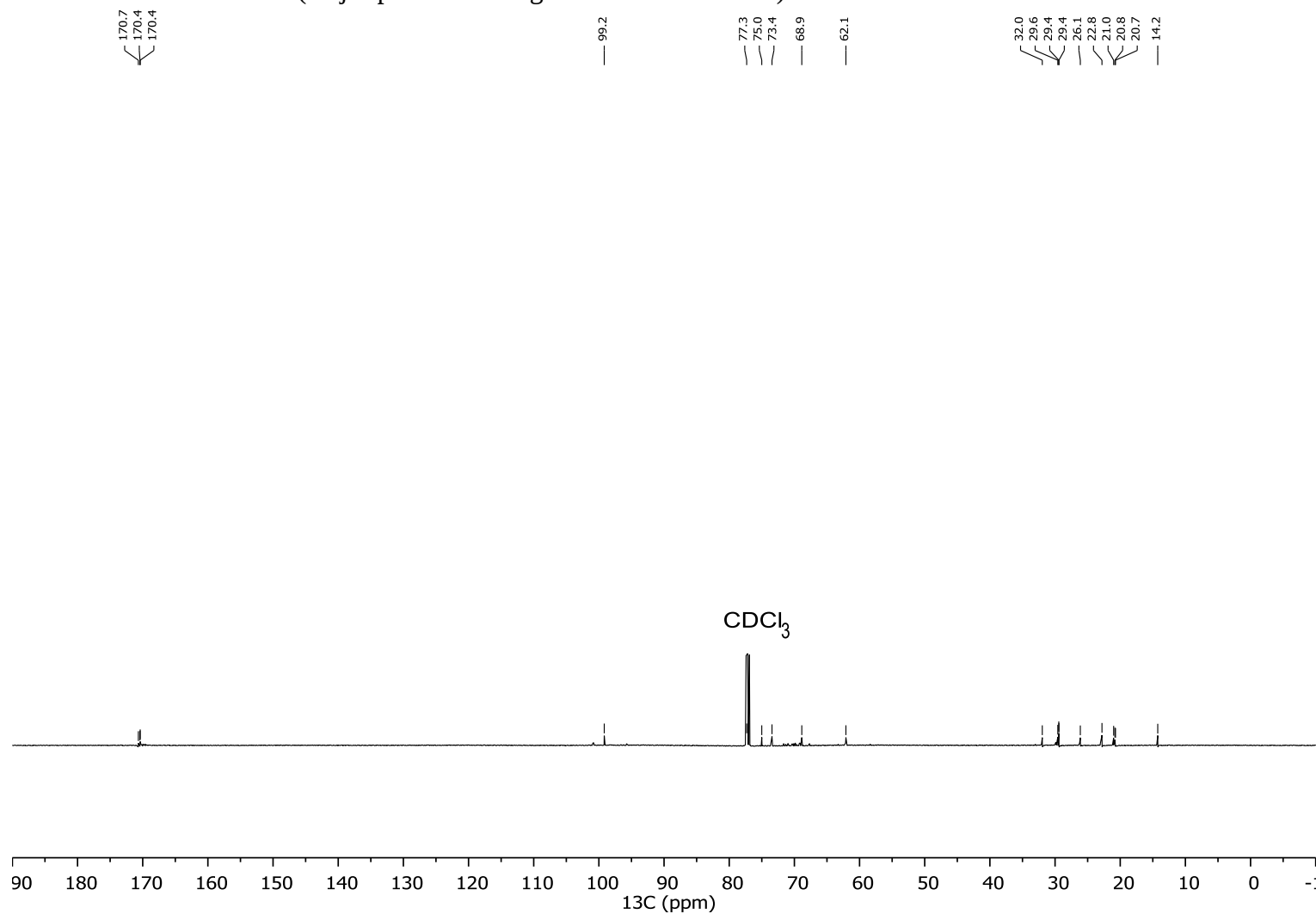
(major product amongst a mixture of isomers)



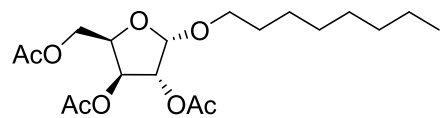
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-xylofuranoside



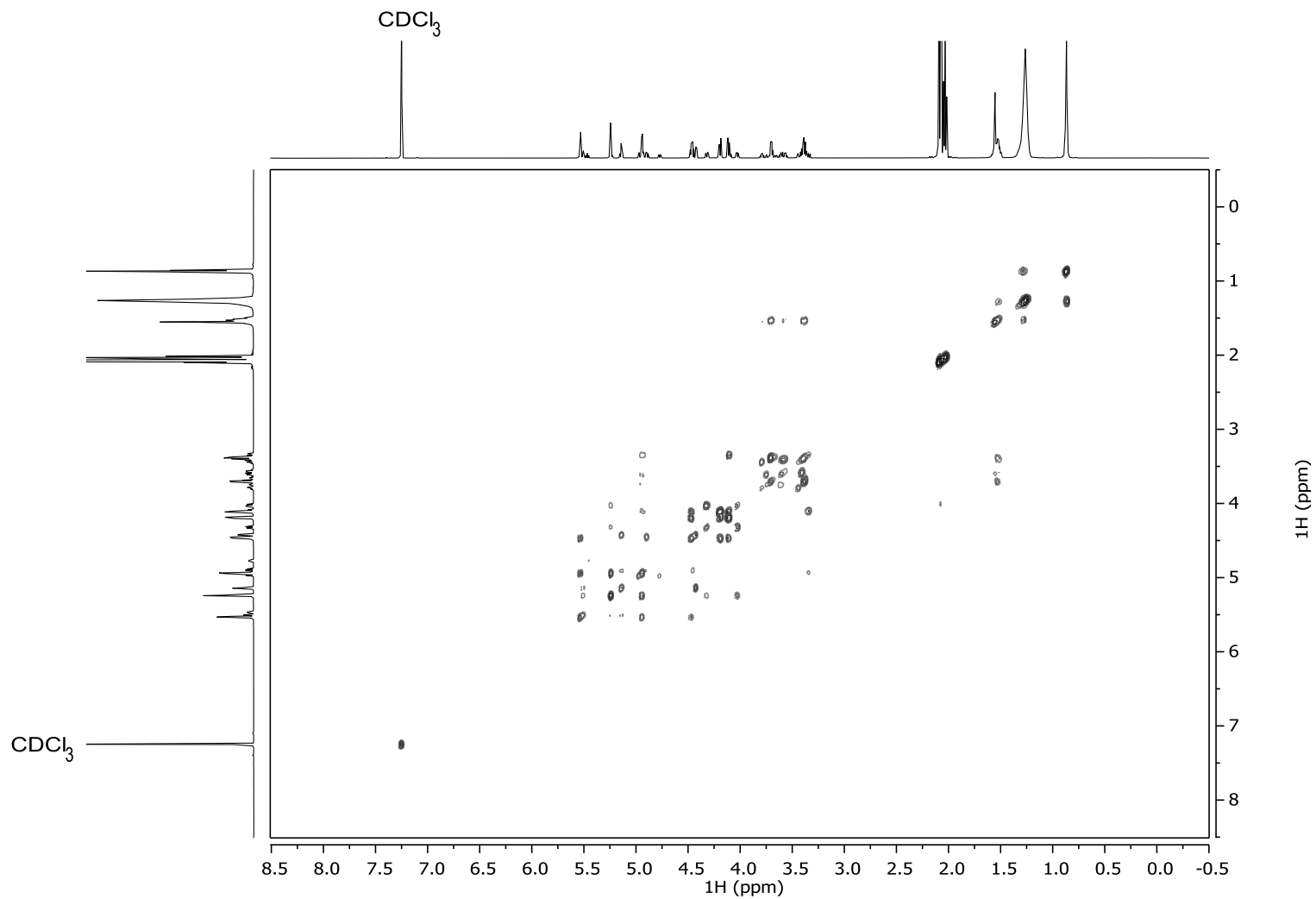
(major product amongst mixture of isomers)



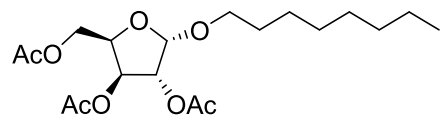
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-xylofuranoside



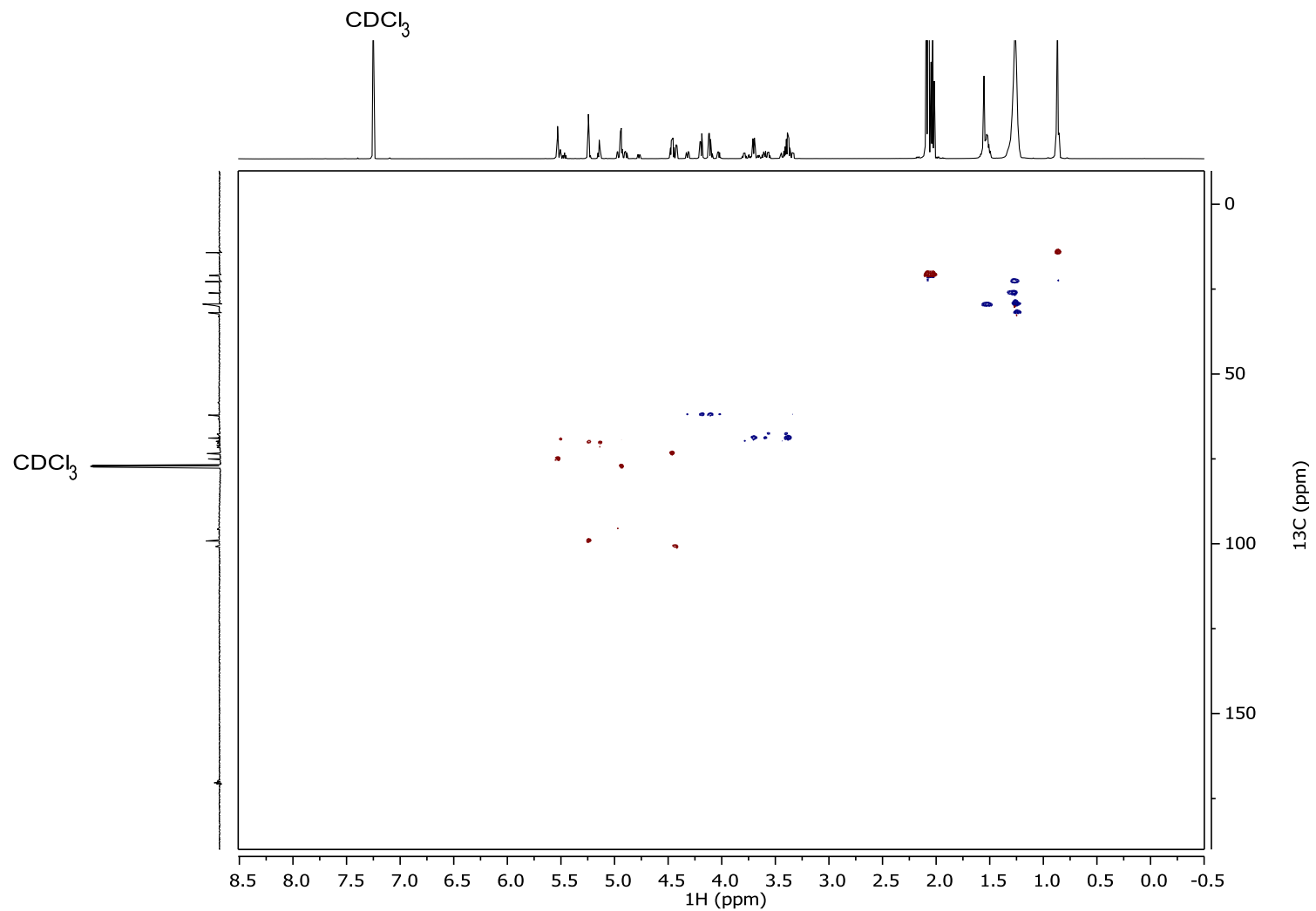
(major product amongst a mixture of isomers)



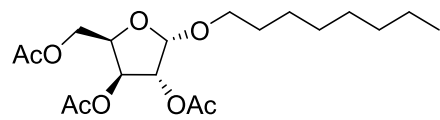
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-xylofuranoside



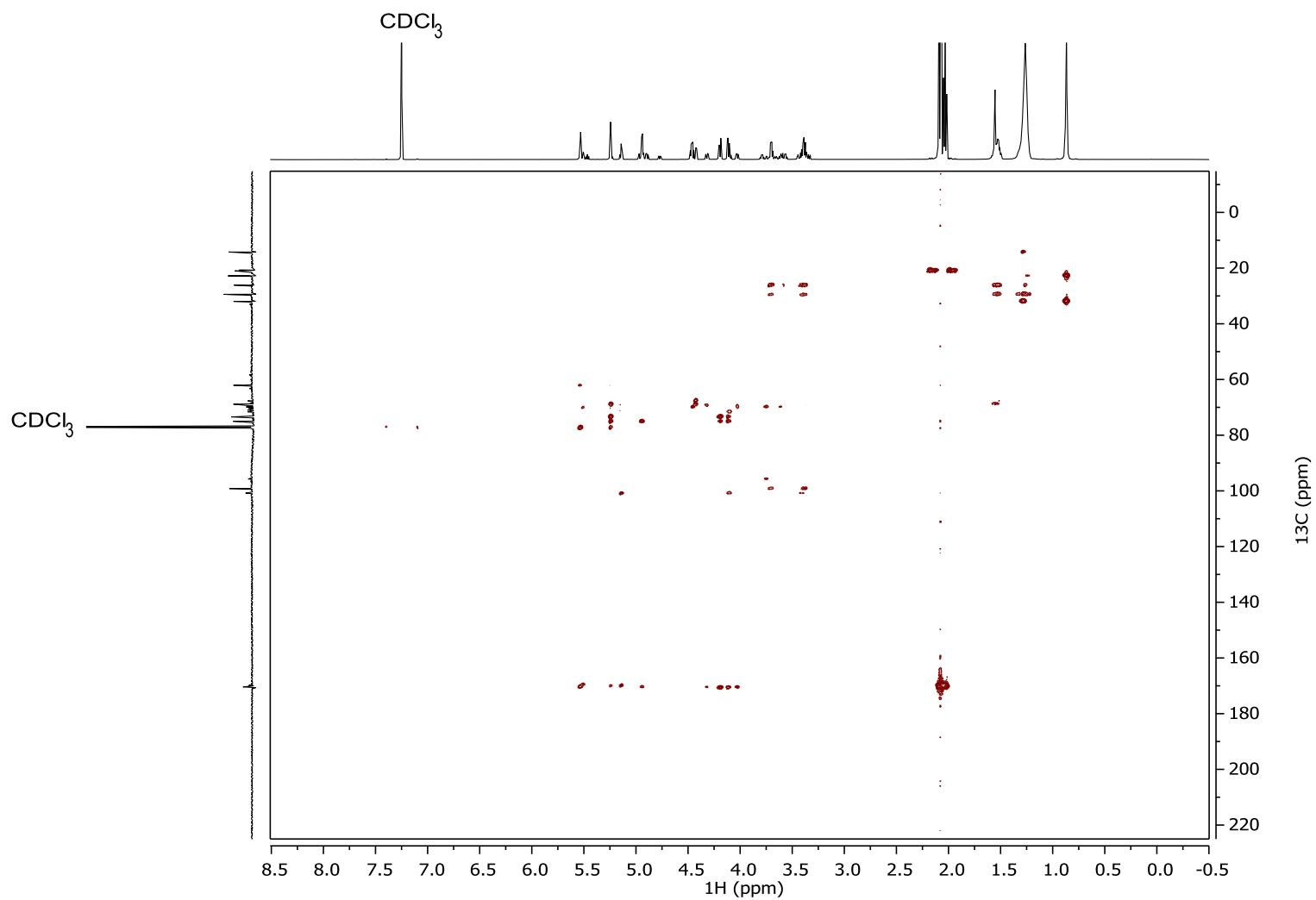
(major product amongst a mixture of isomers)



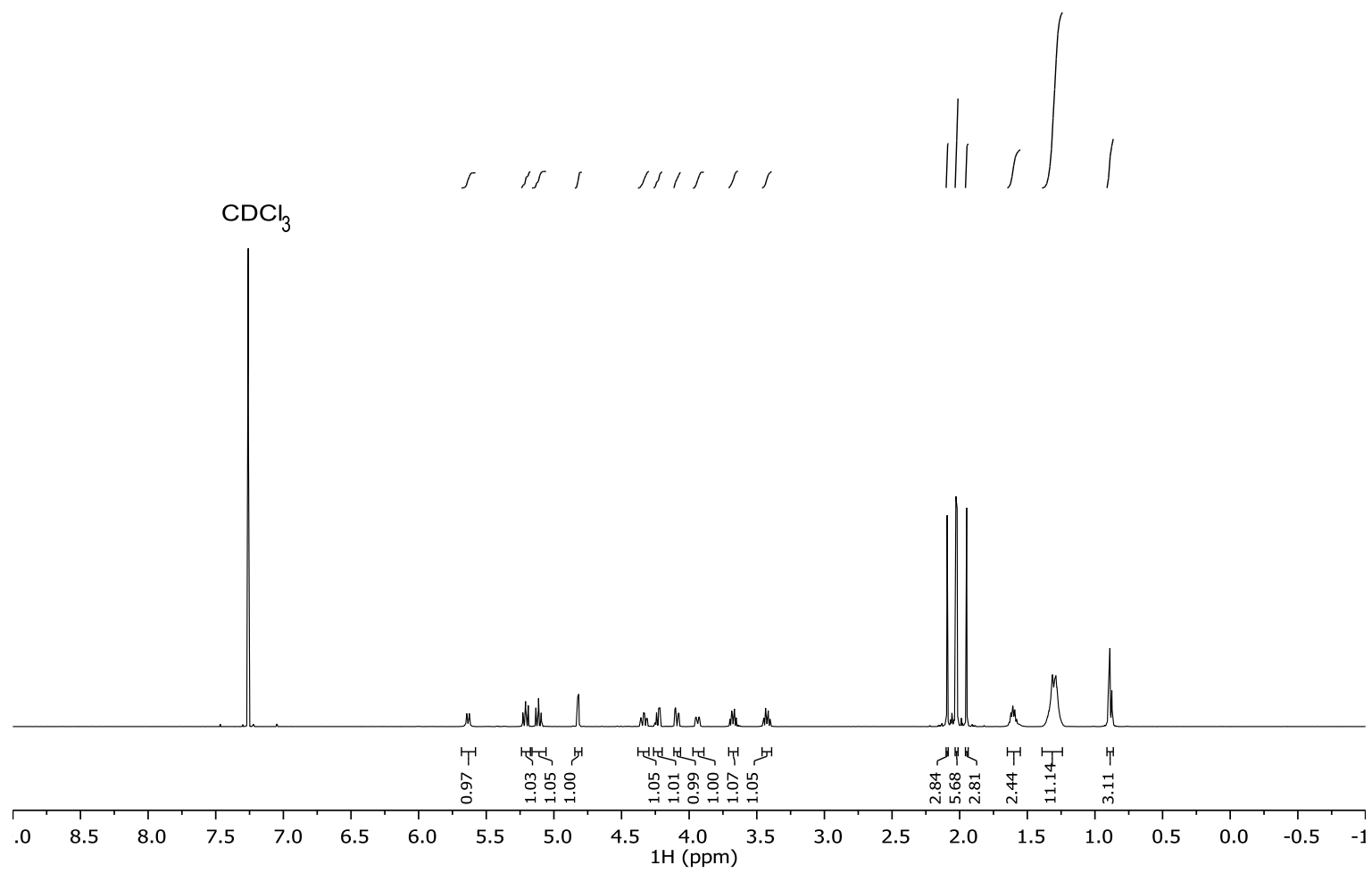
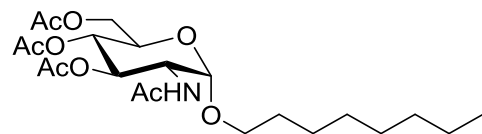
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl 2,3,5-tri-*O*-acetyl- α -D-xylofuranoside



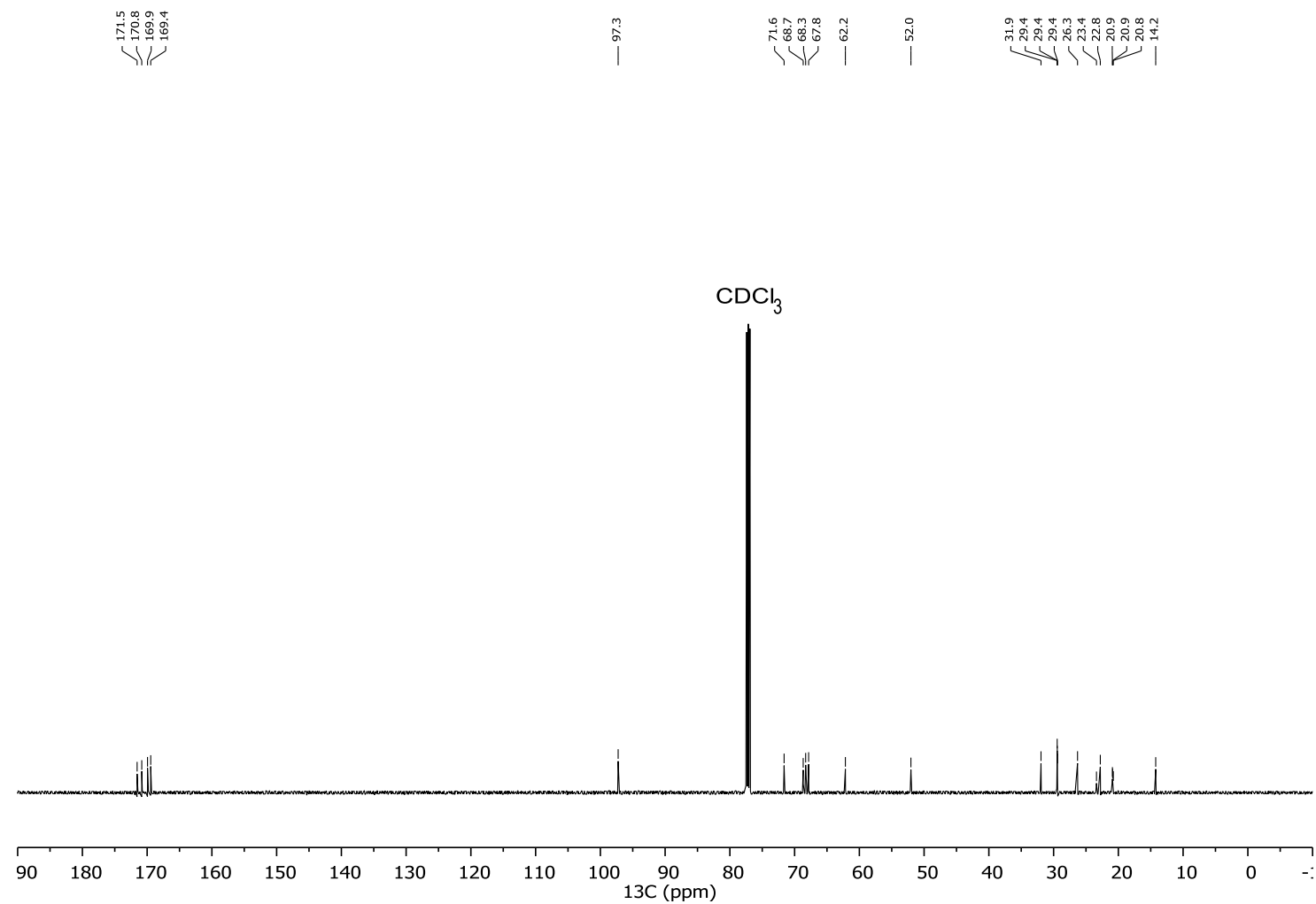
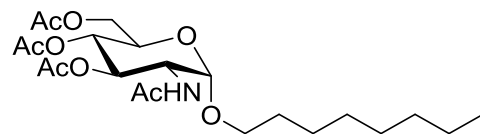
(major product amongst a mixture of isomers)



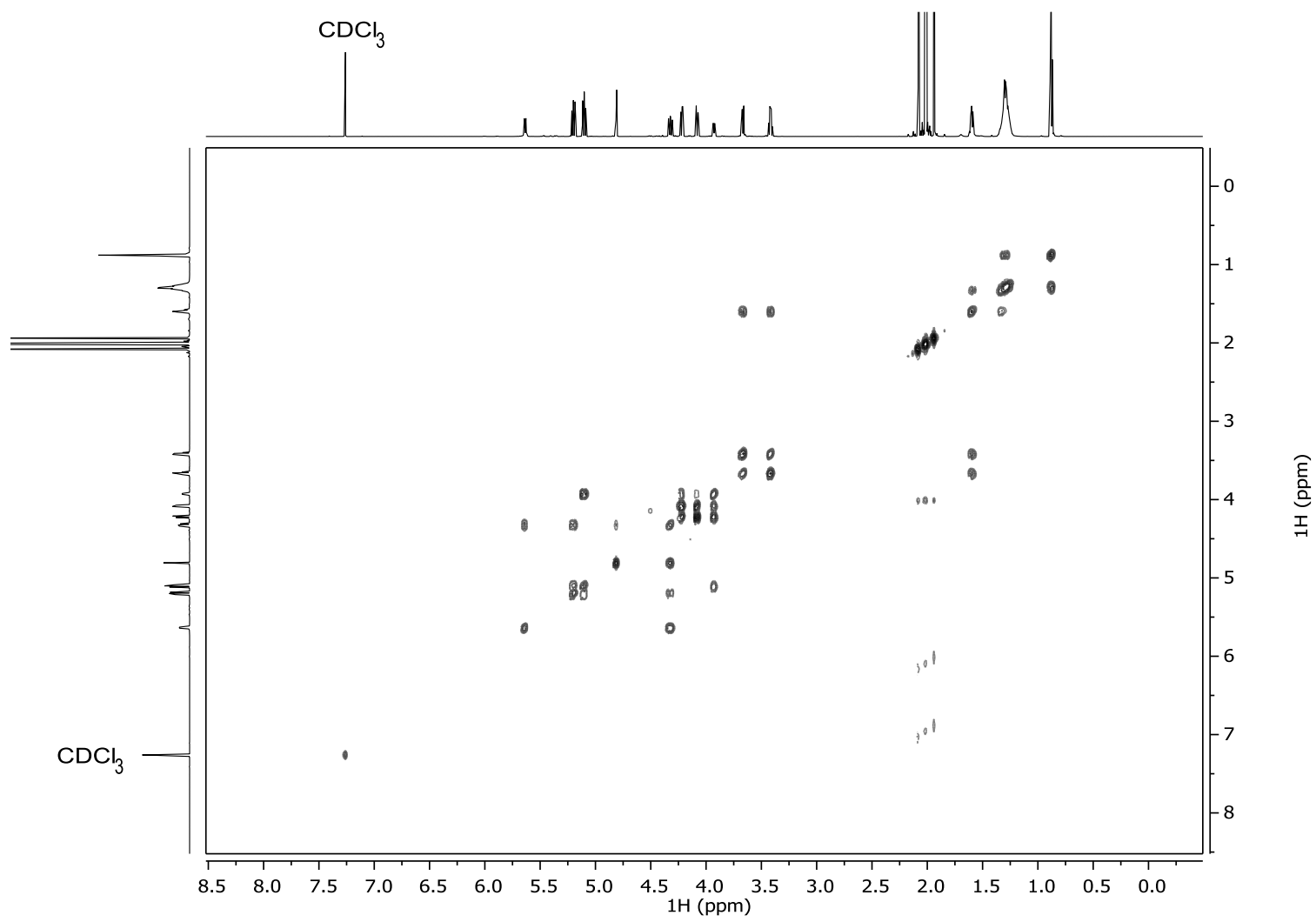
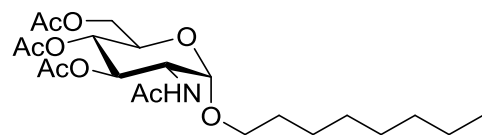
^1H NMR (500 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,4,6-tri-*O*-acetyl- α -D-glucopyranoside



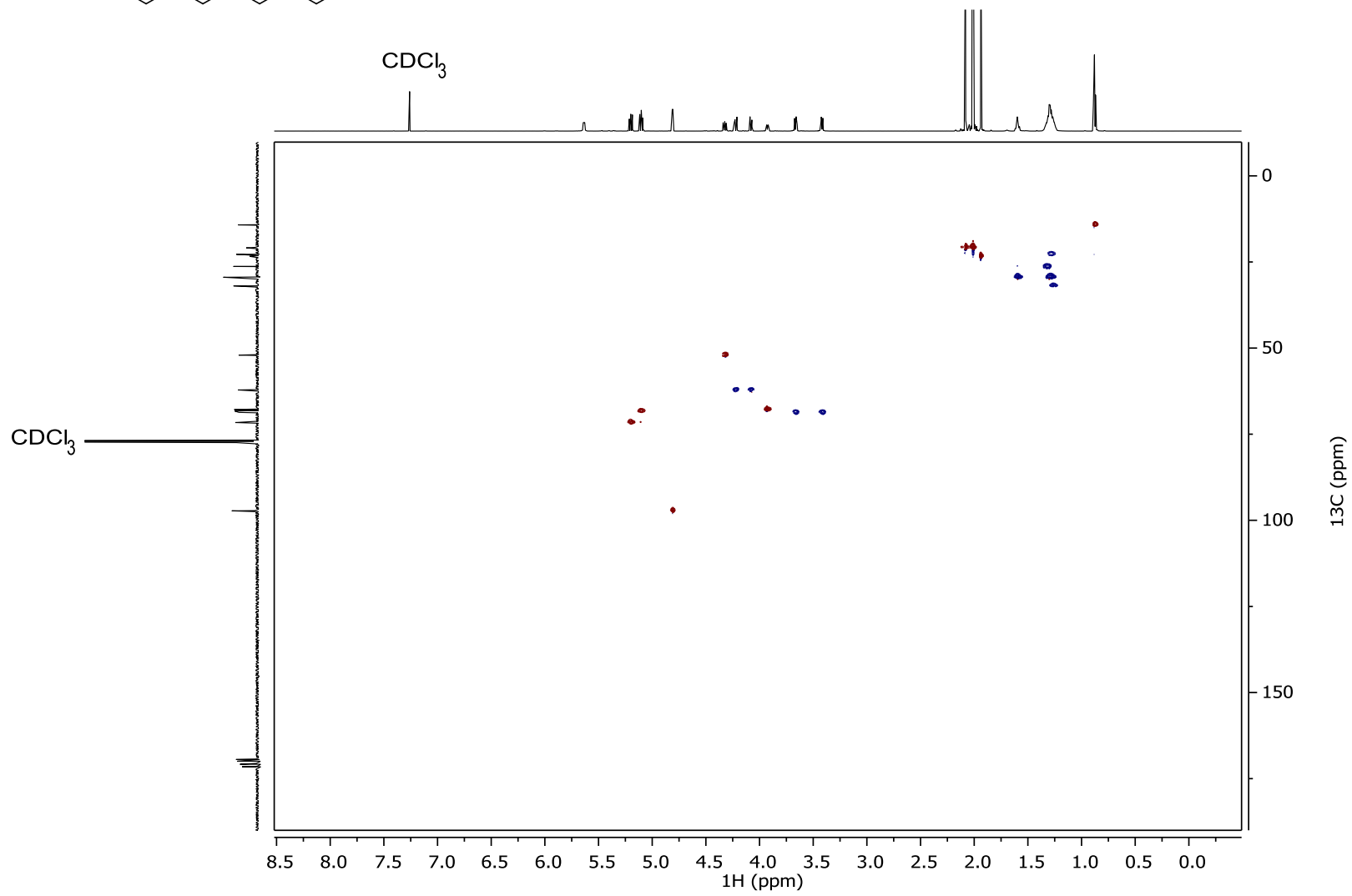
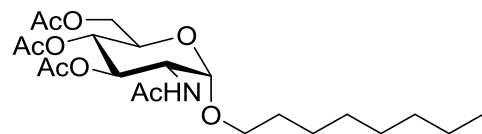
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,4,6-tri-*O*-acetyl- α -D-glucopyranoside



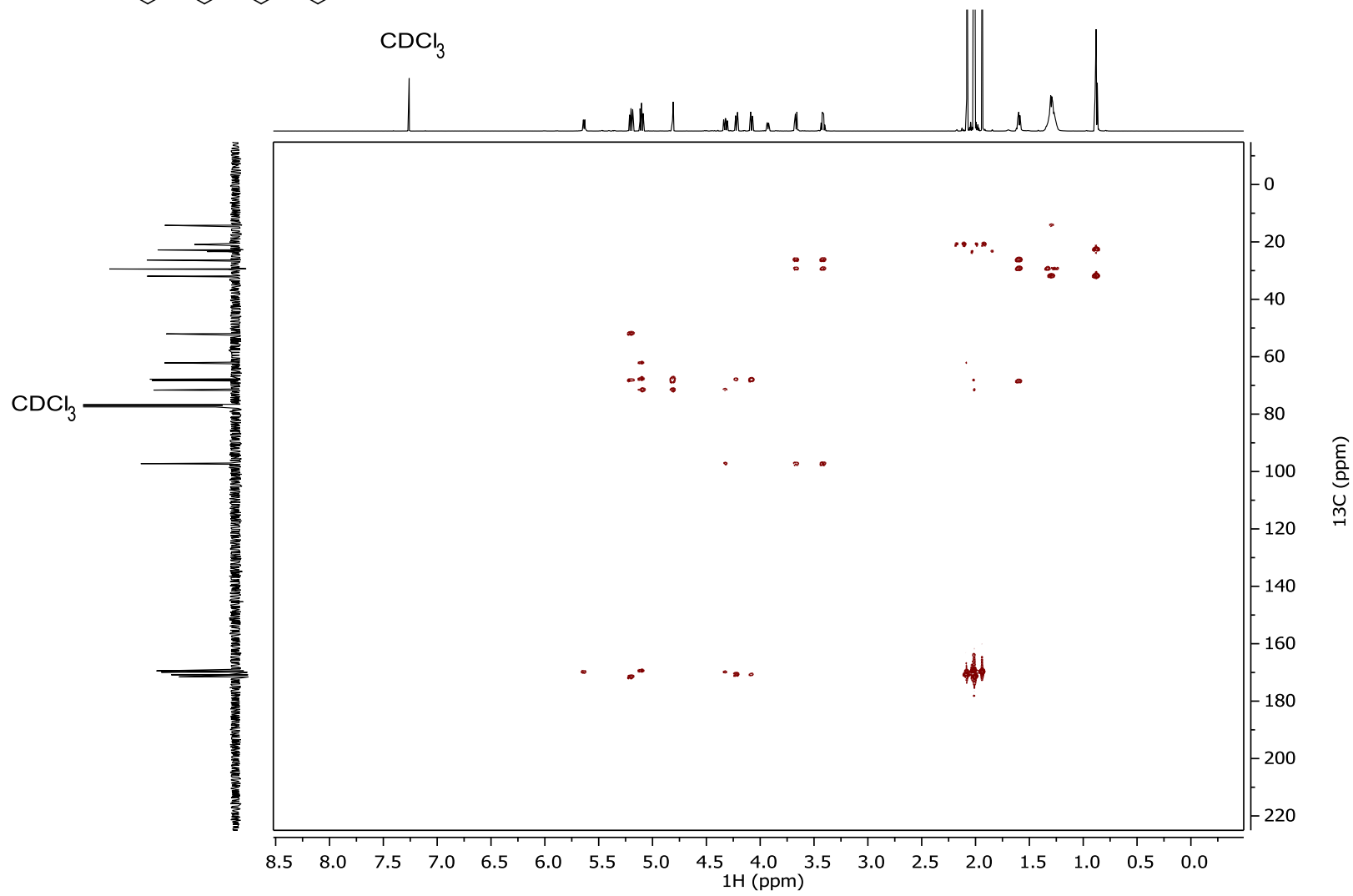
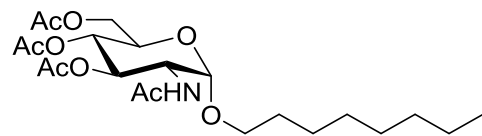
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,4,6-tri-*O*-acetyl- α -D-glucopyranoside



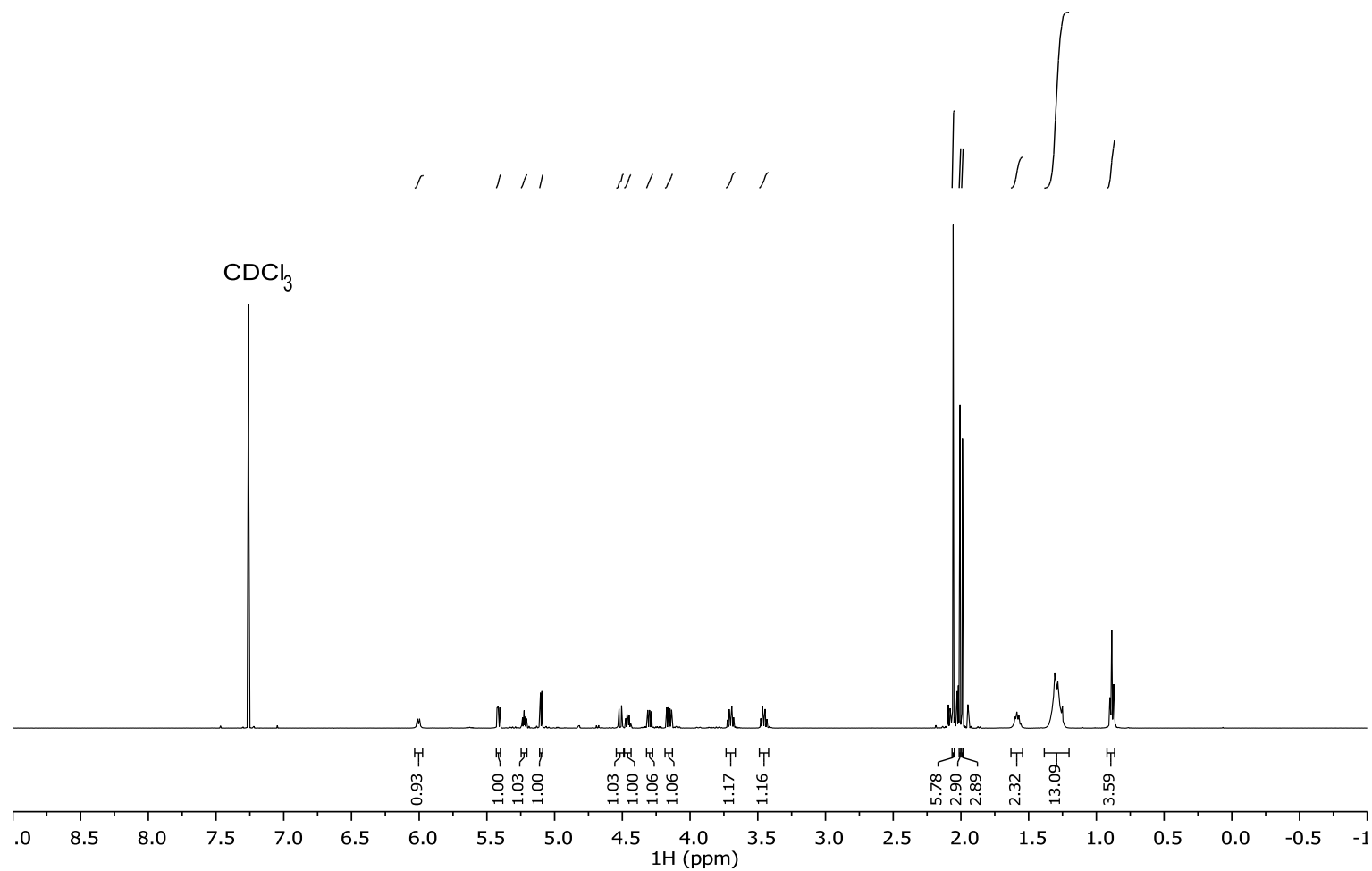
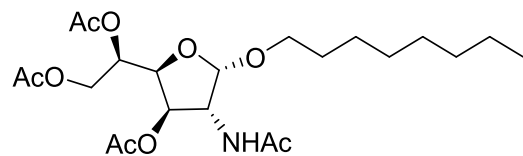
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,4,6-tri-*O*-acetyl- α -D-glucopyranoside



^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,4,6-tri-*O*-acetyl- α -D-glucopyranoside

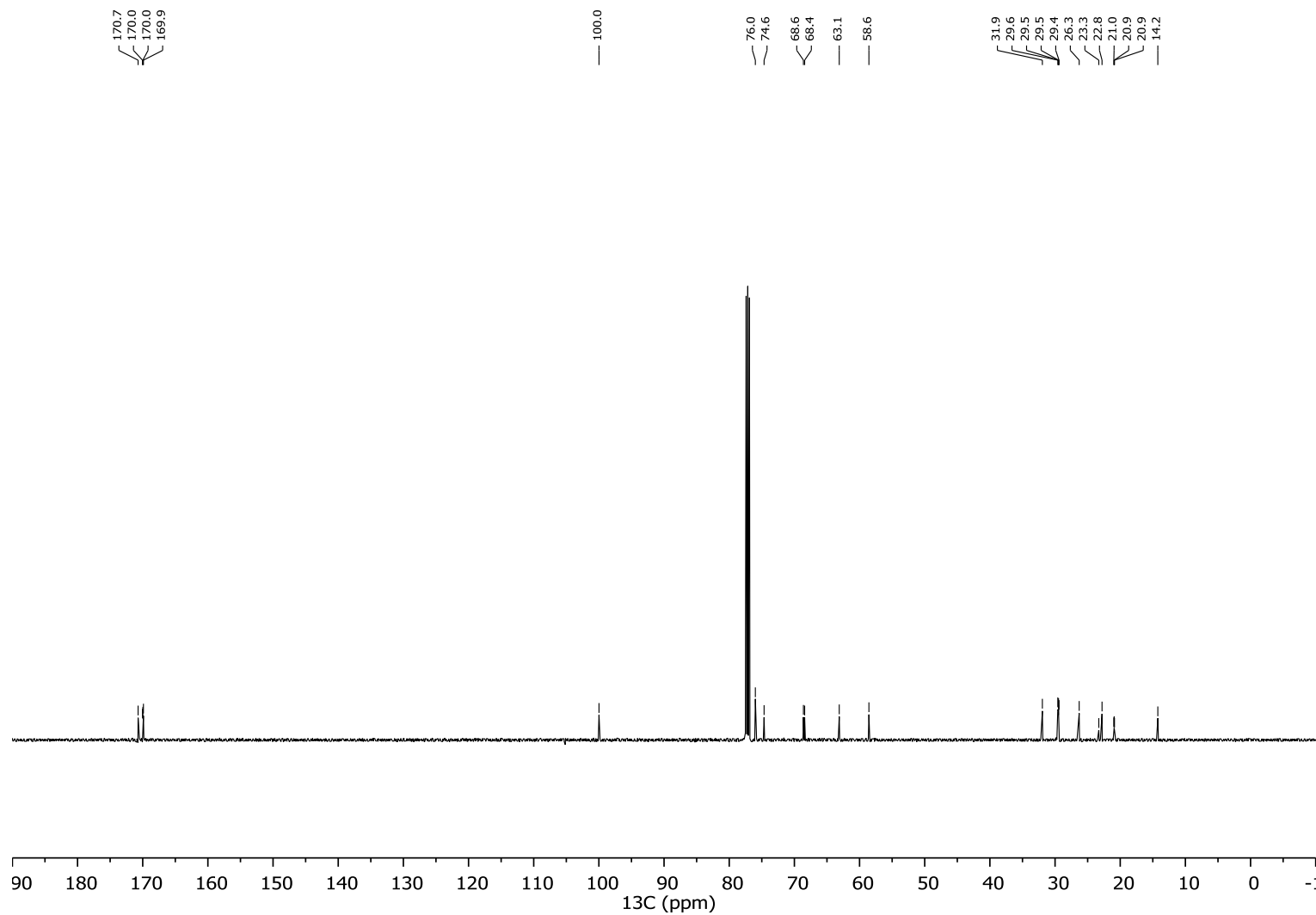
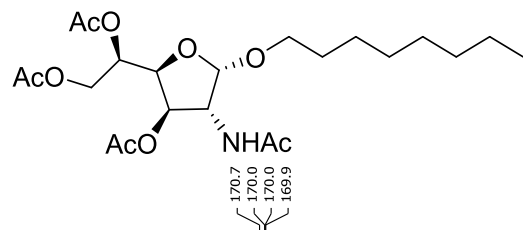


^1H NMR (500 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- α -D-glucofuranoside

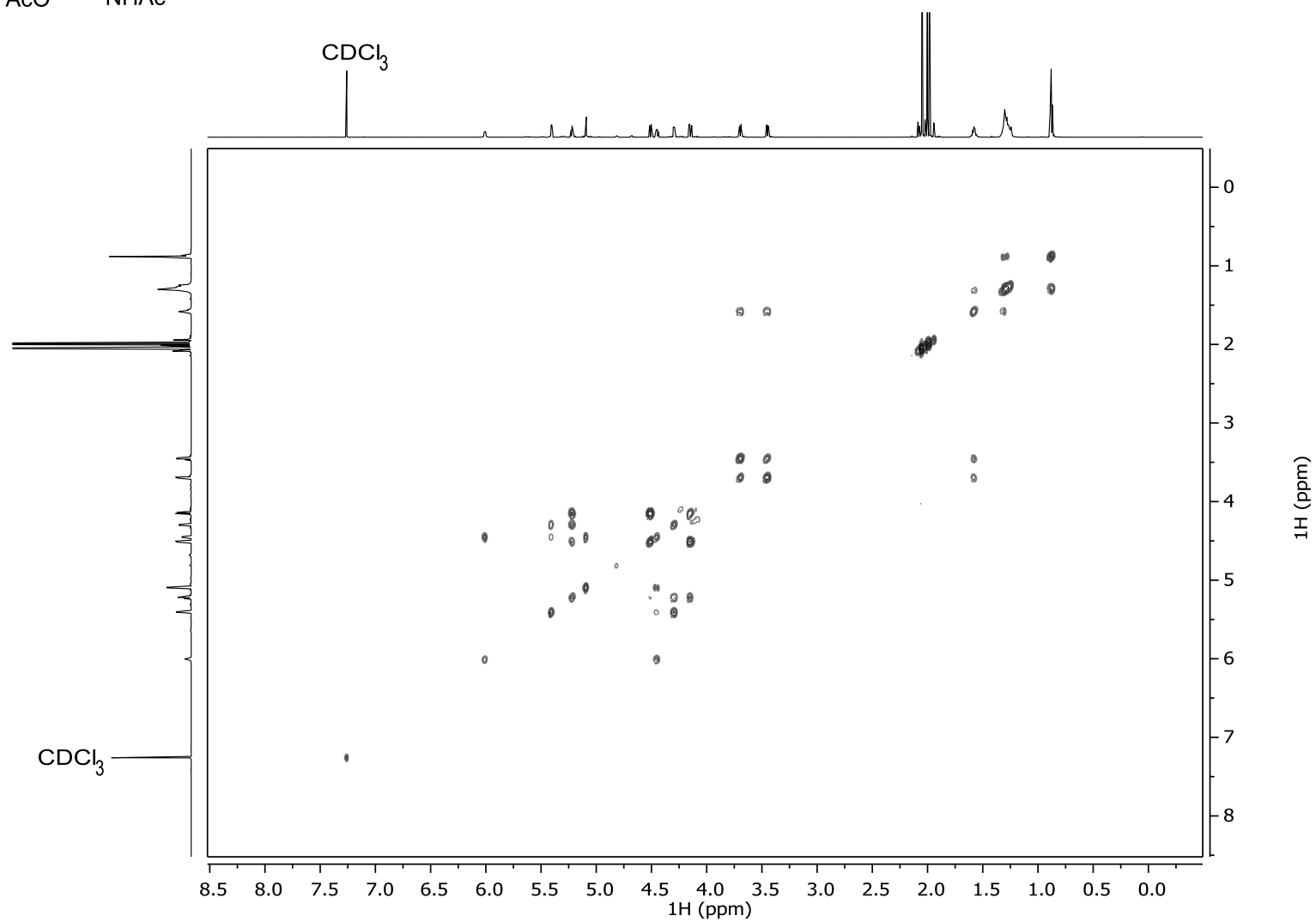
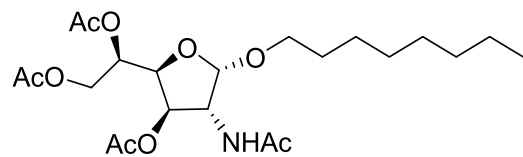


S117

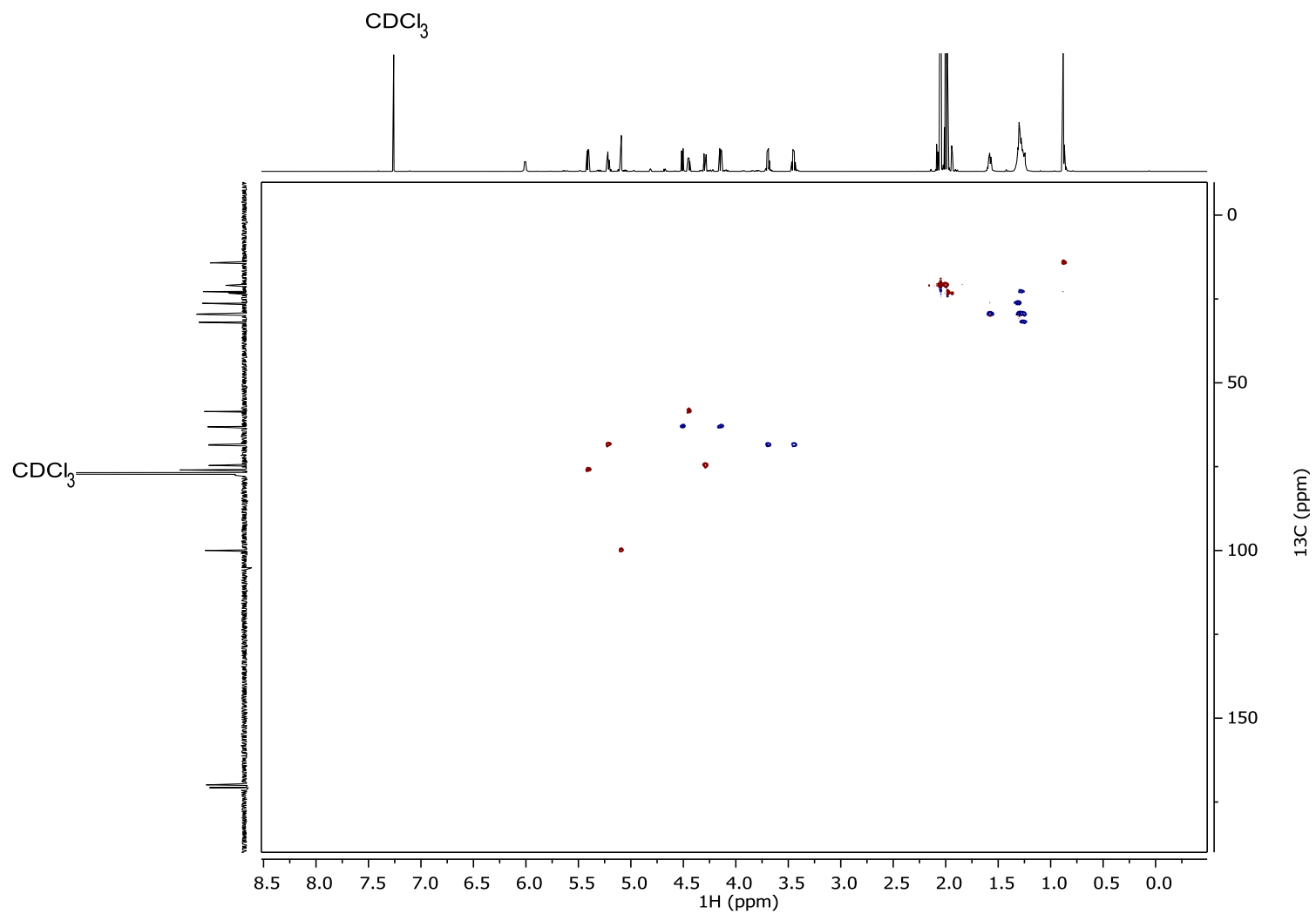
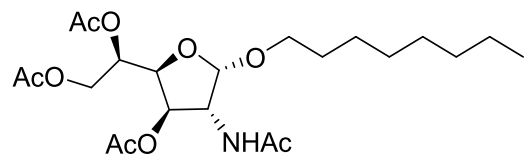
^{13}C NMR (126 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- α -D-glucofuranoside



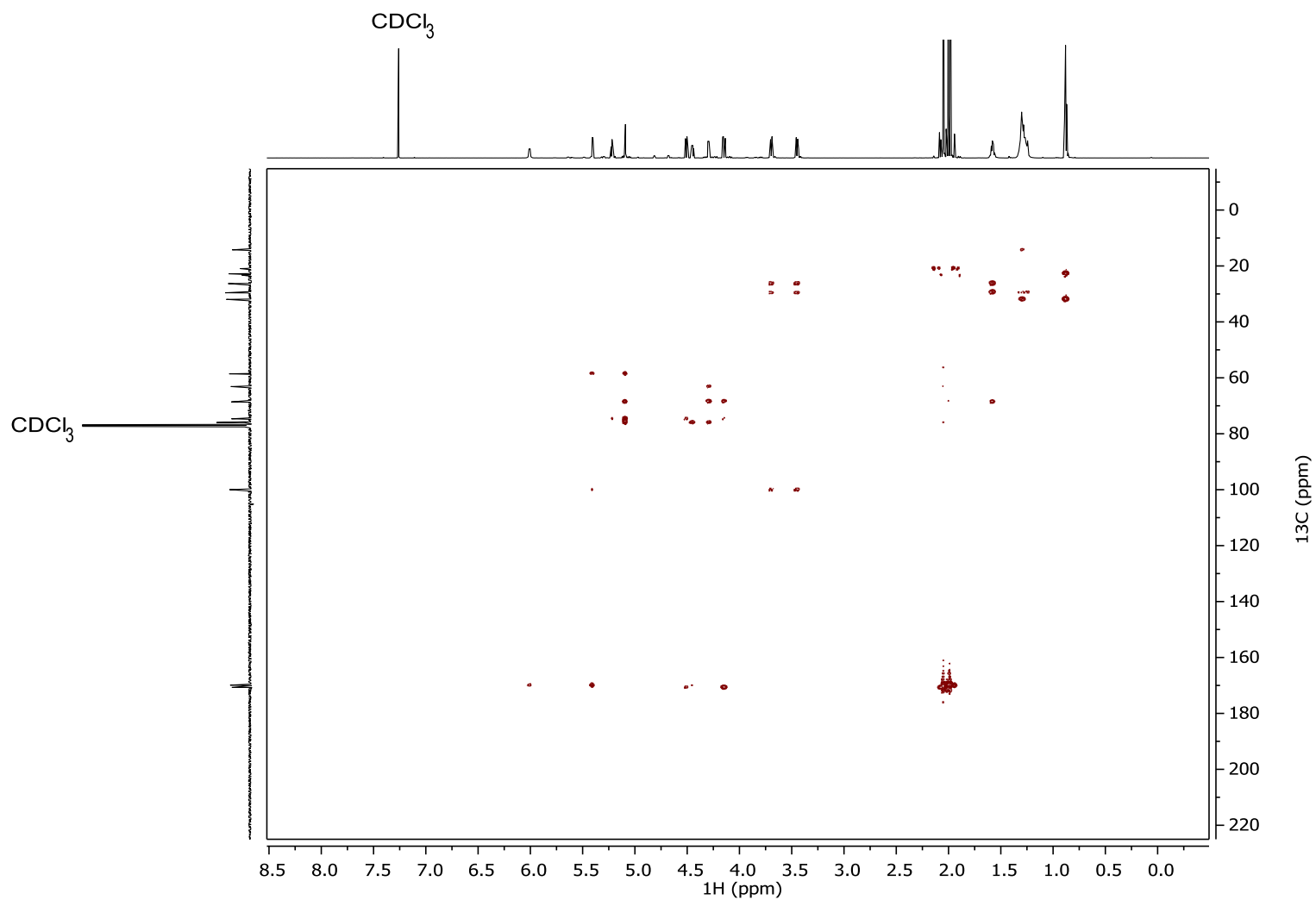
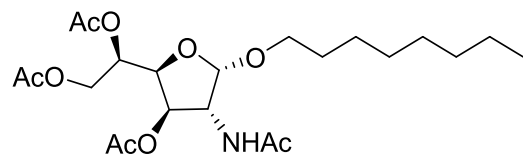
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- α -D-glucopyranoside



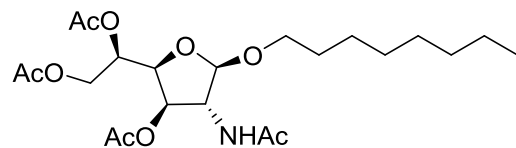
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- α -D-glucopyranoside



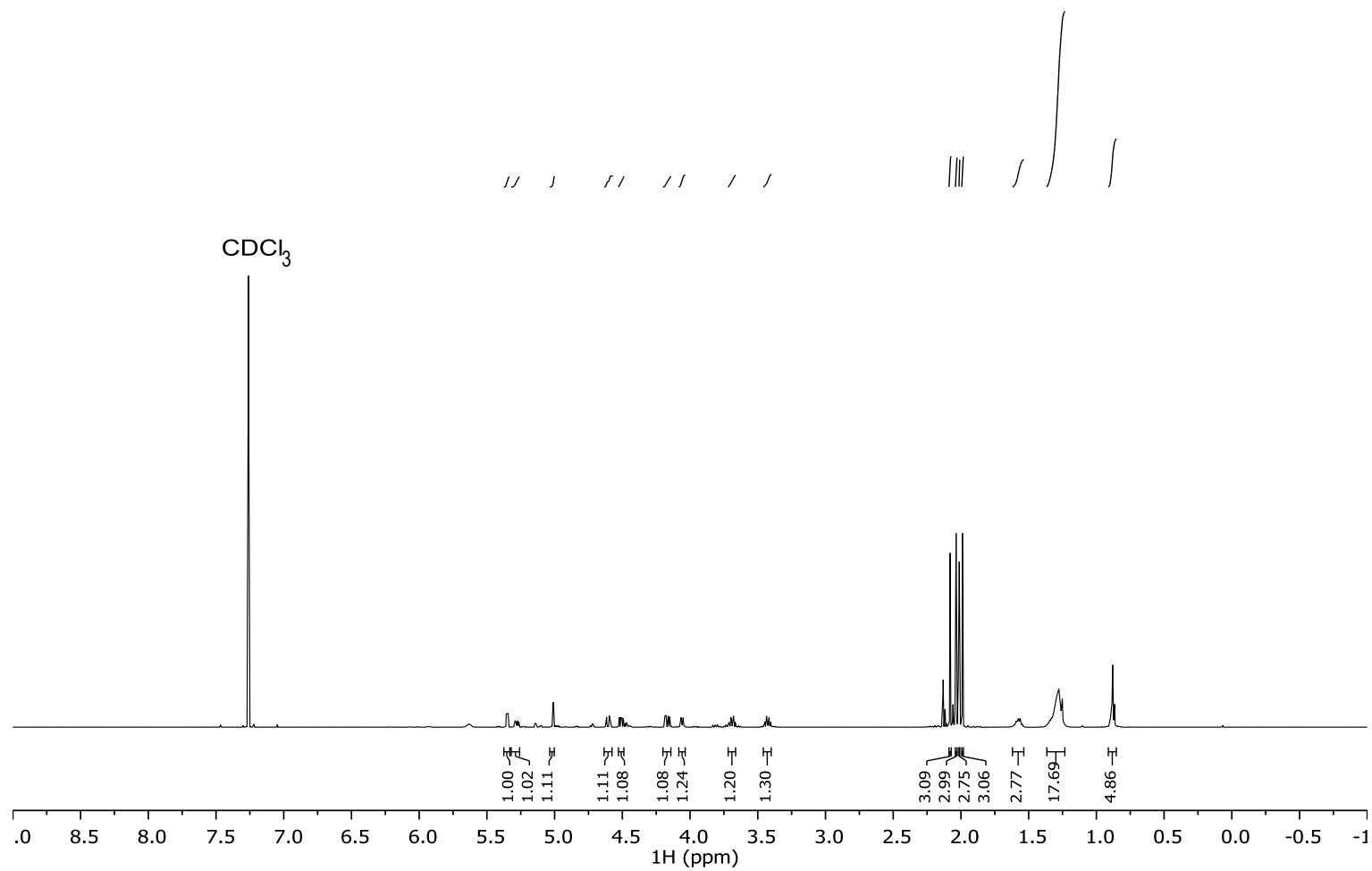
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- α -D-glucofuranoside



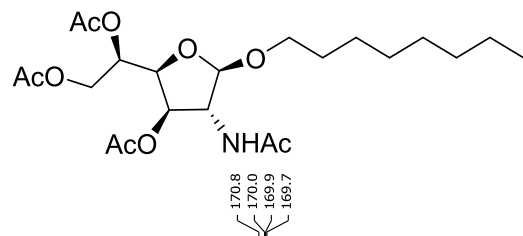
^1H NMR (500 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- β -D-glucopyranoside



(major product amongst a mixture of isomers)



^{13}C NMR (126 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- β -D-glucofuranoside



(major product amongst a mixture of isomers)

106.7

75.2

69.2

69.1

63.4

62.2

32.0

29.7

29.5

29.4

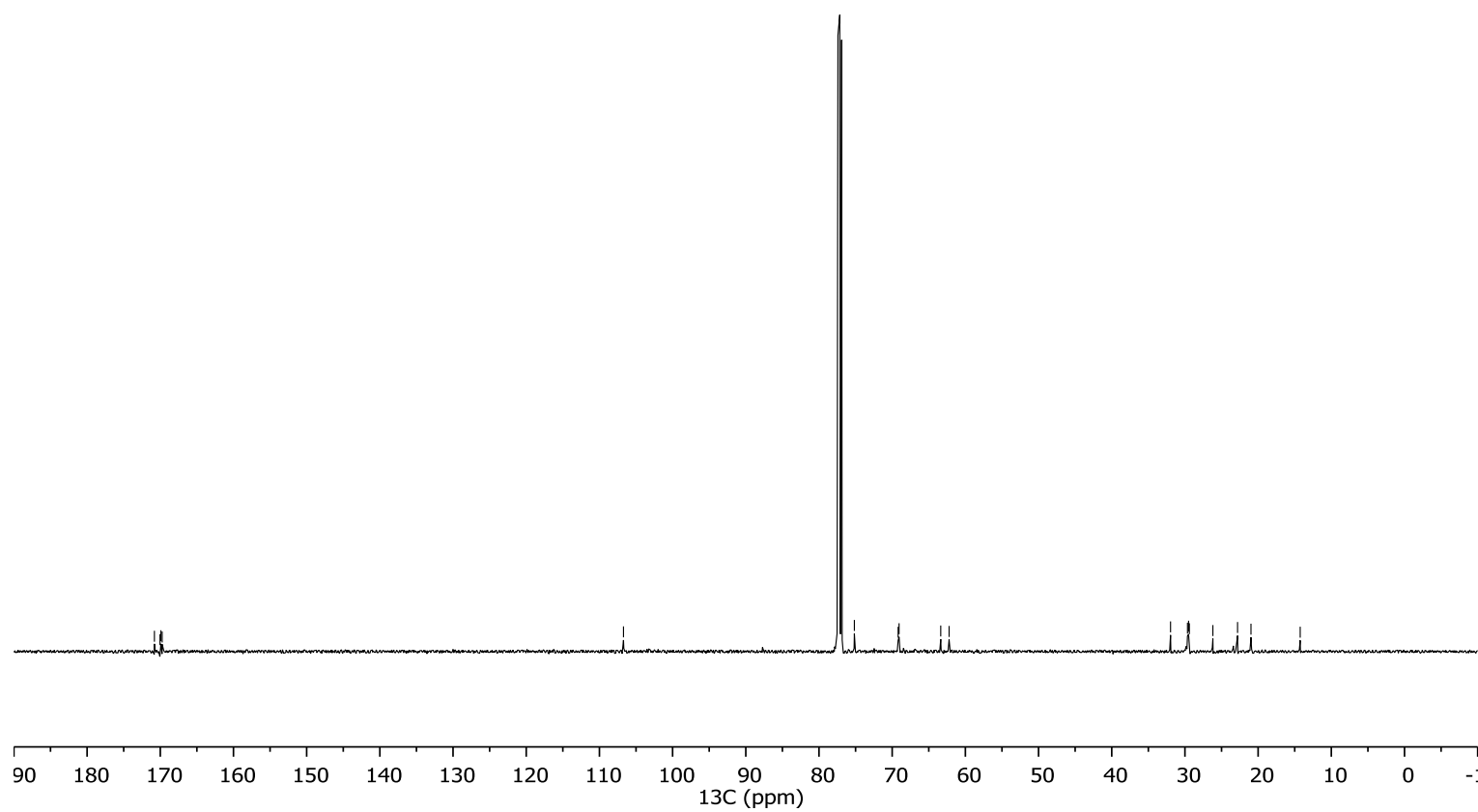
26.2

22.8

21.0

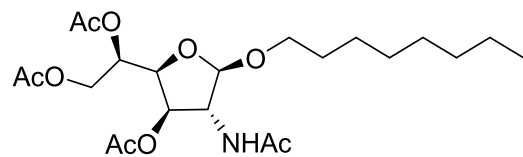
14.3

CDCl_3

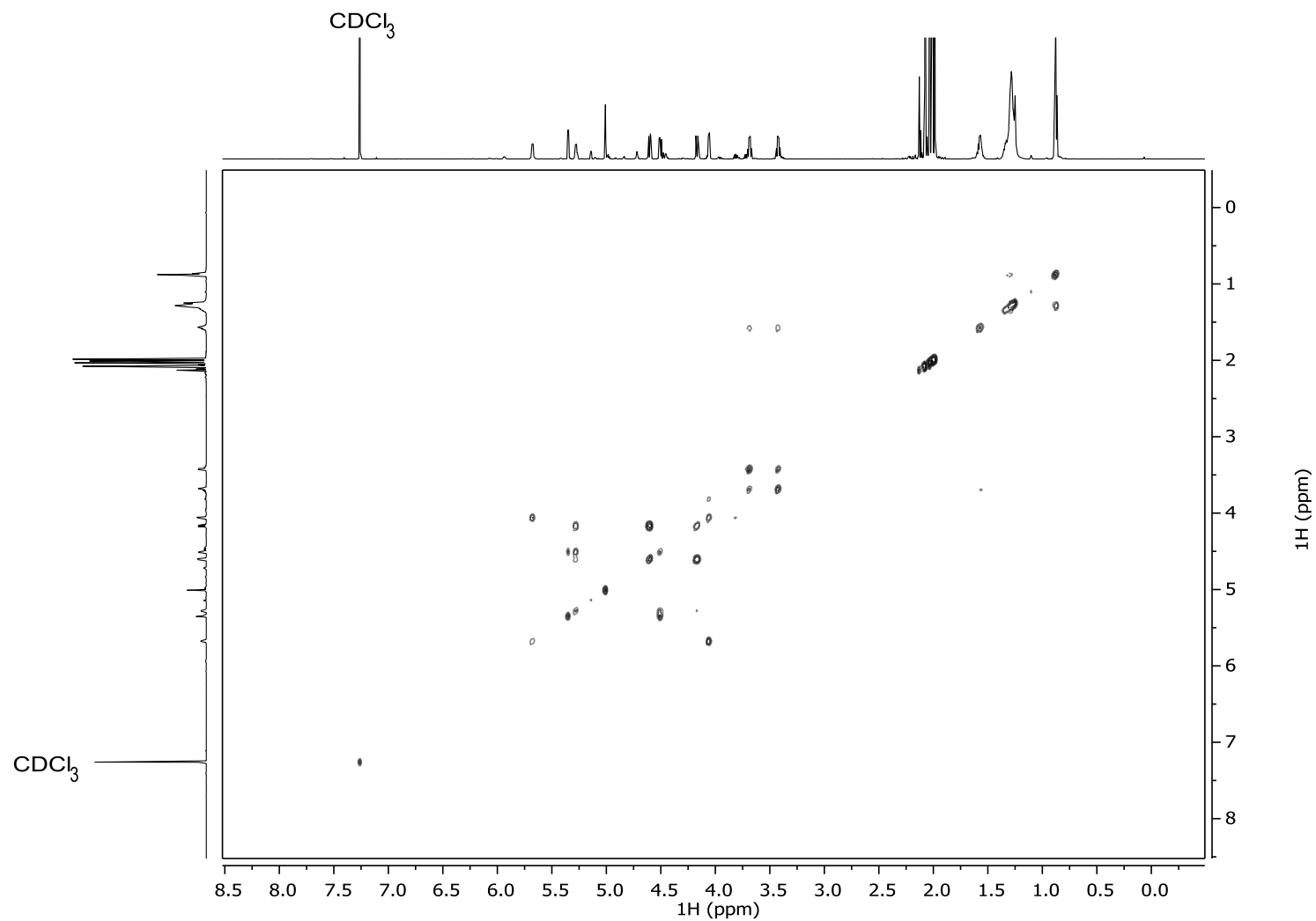


S123

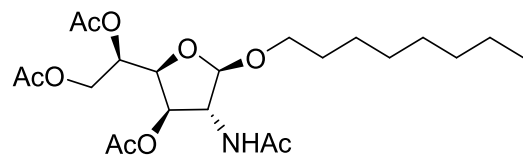
^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- β -D-glucofuranoside



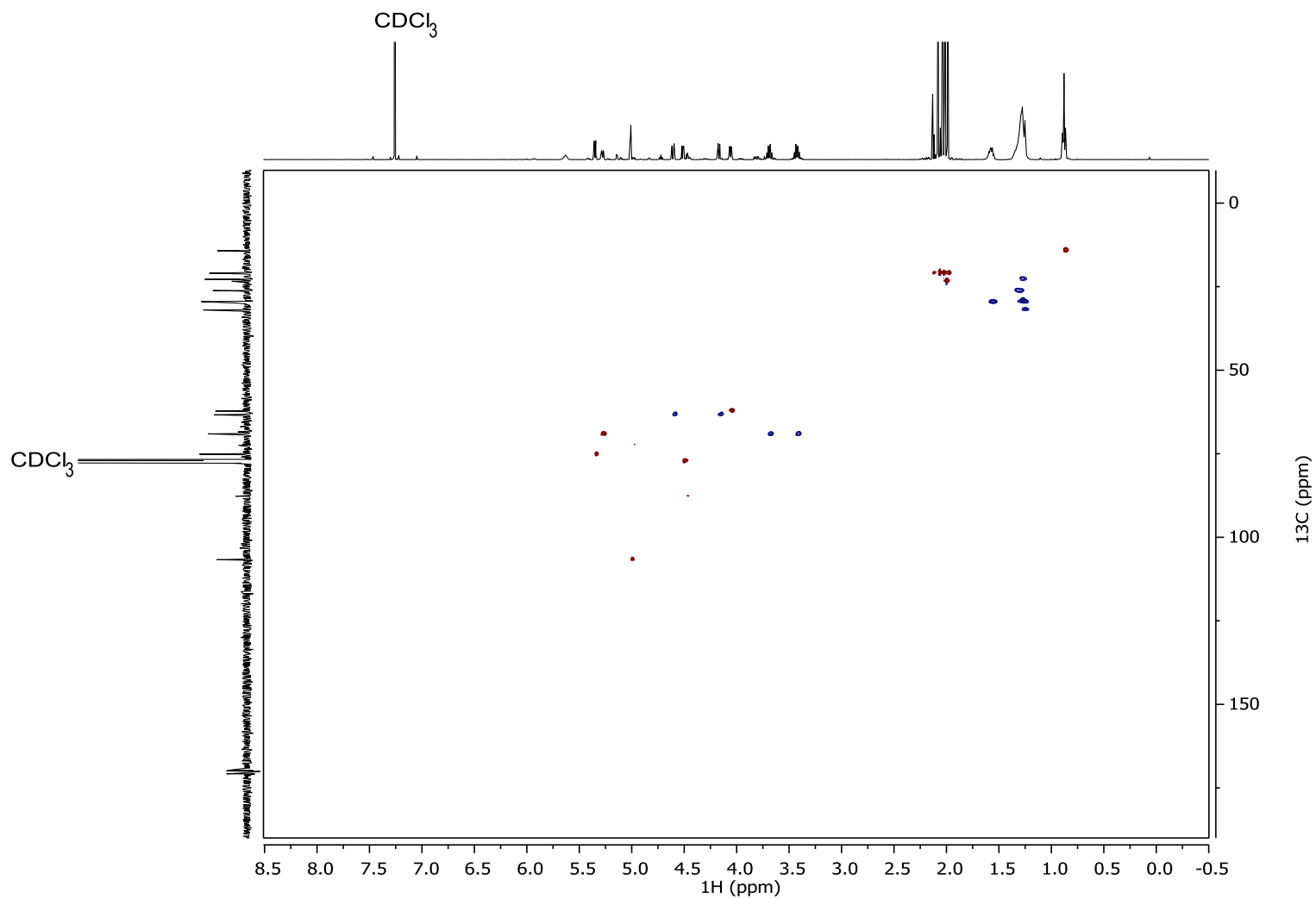
(major product amongst a mixture of isomers)



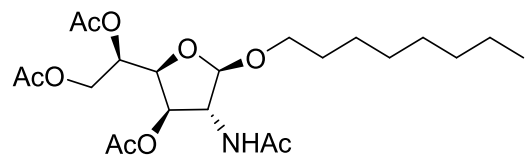
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- β -D-glucofuranoside



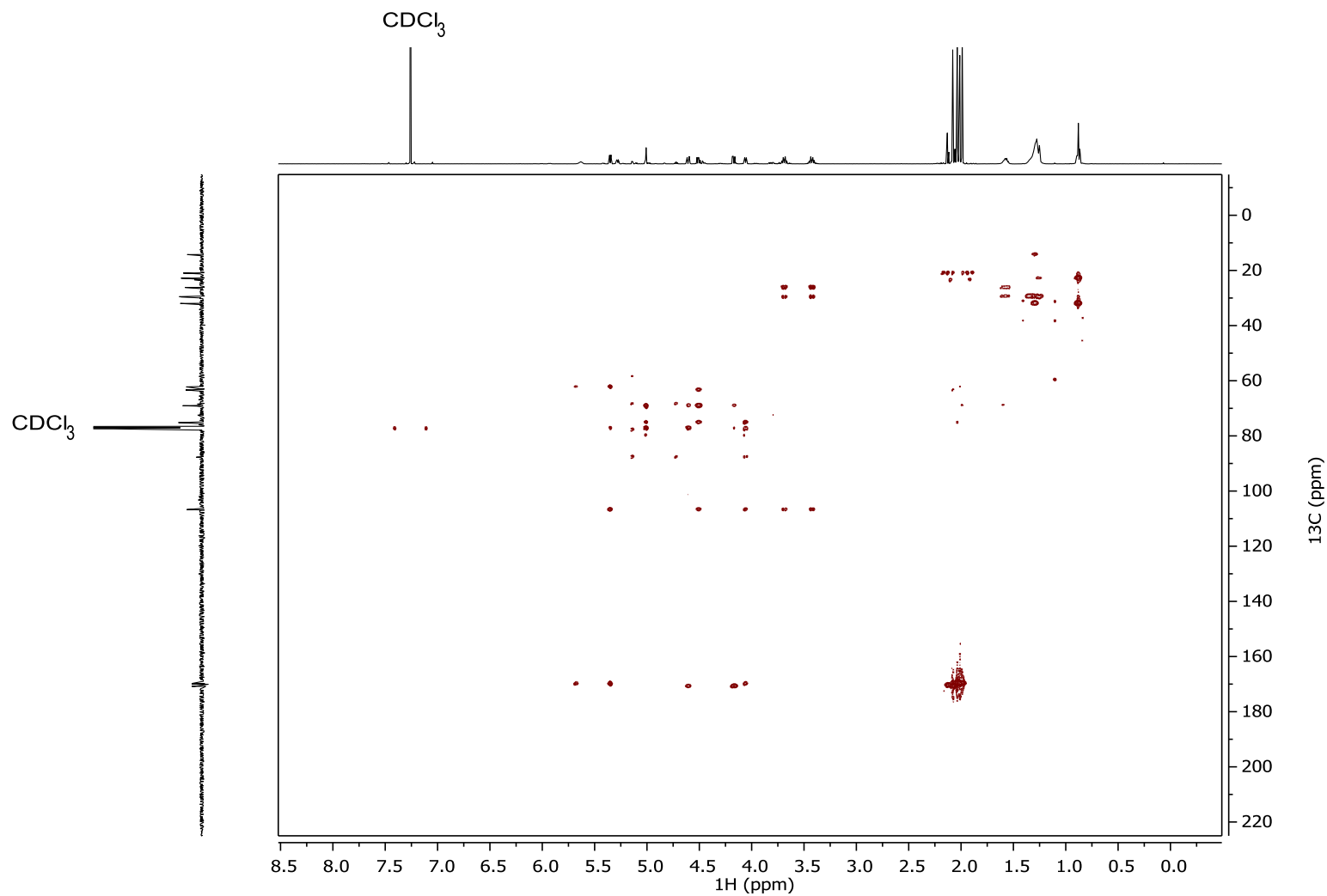
(major product amongst a mixture of isomers)



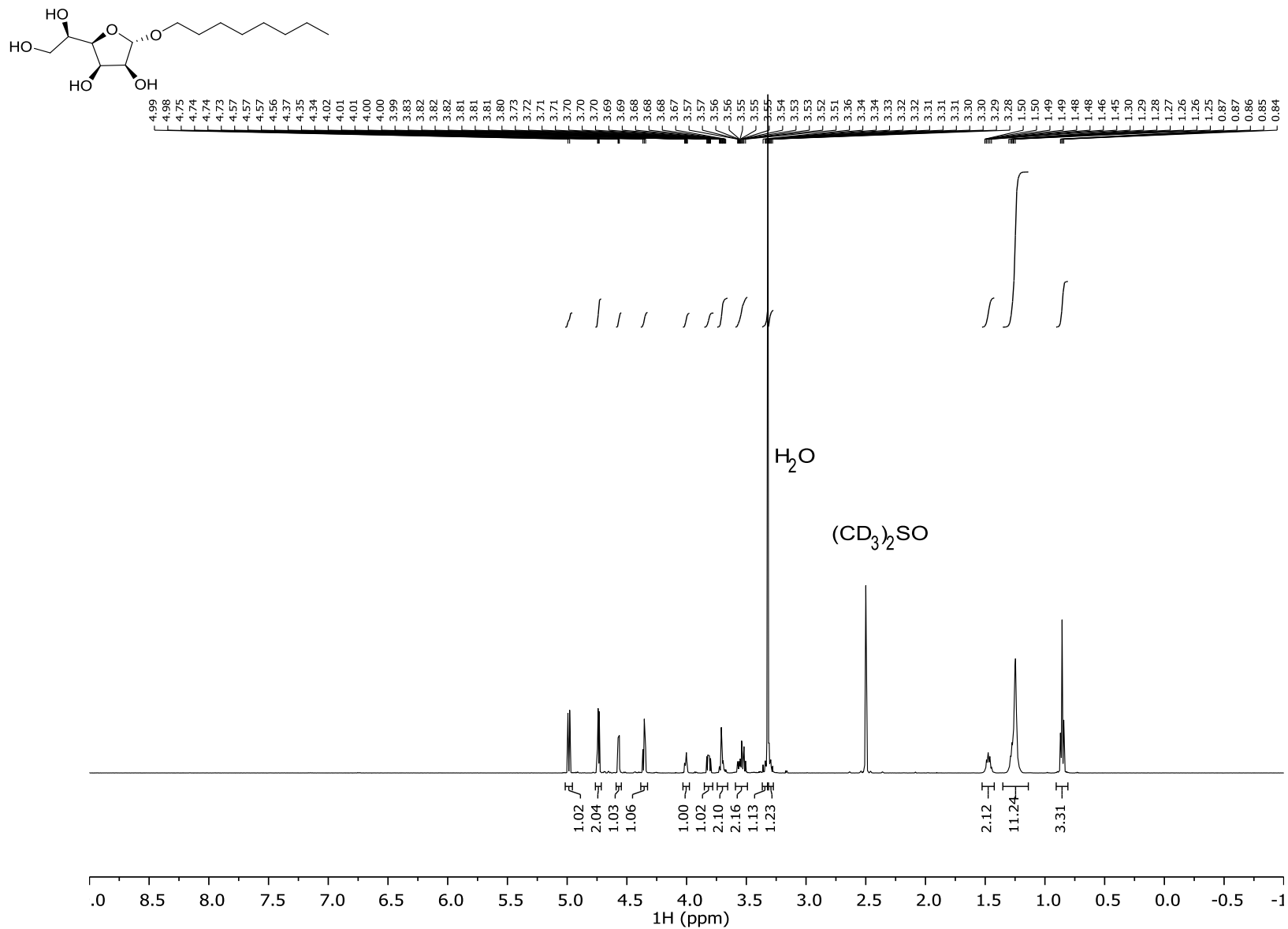
^1H - ^{13}C HMBC NMR (700 MHz, CDCl_3) *n*-octyl-2-acetamido-2-deoxy-3,5,6-tri-*O*-acetyl- β -D-glucofuranoside



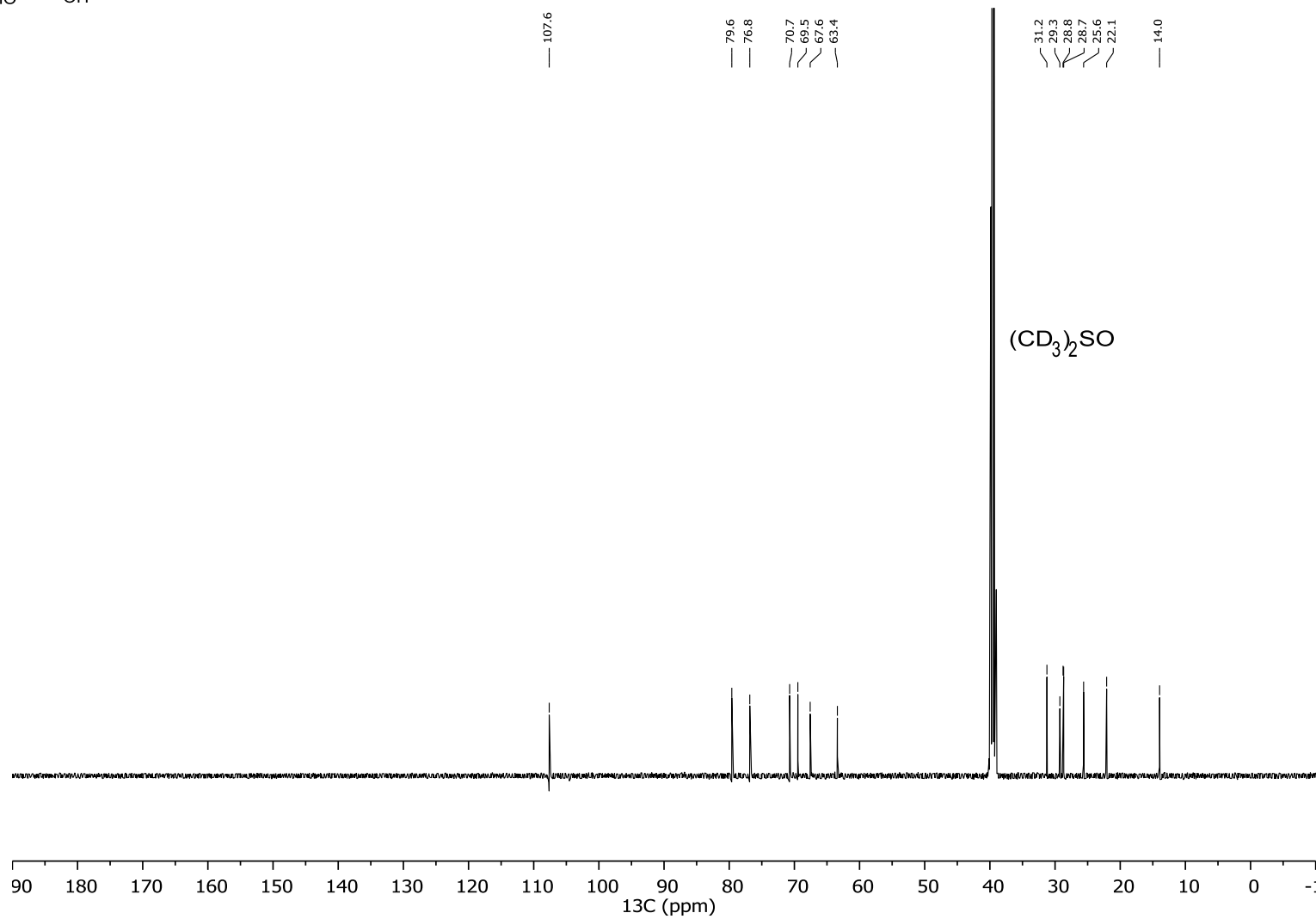
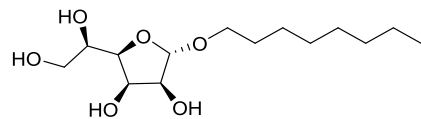
(major product amongst a mixture of isomers)



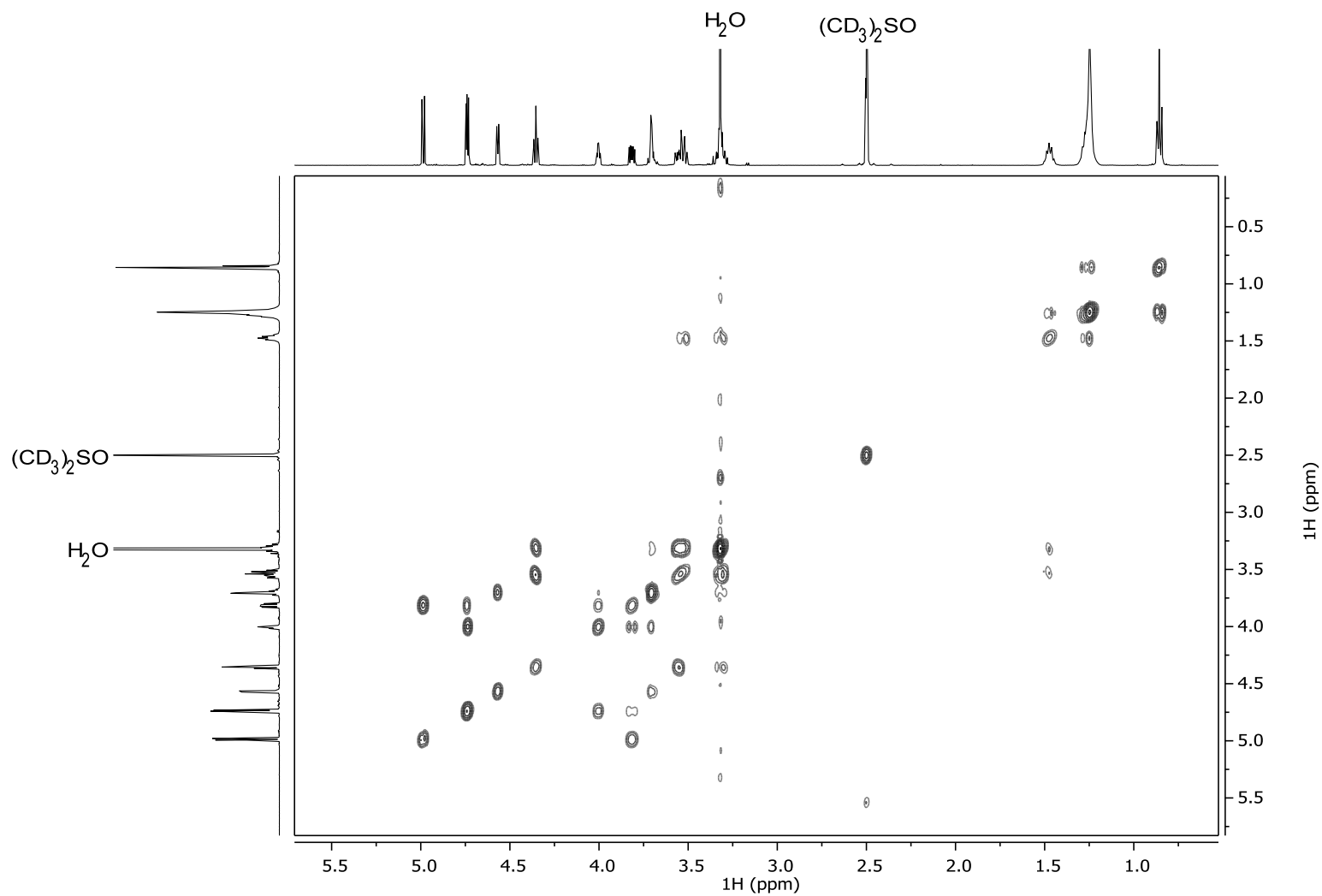
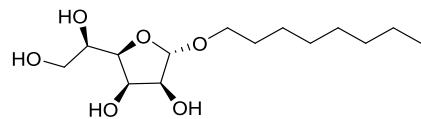
^1H NMR (500 MHz, DMSO- d_6) *n*-octyl- α -D-mannofuranoside (3a)



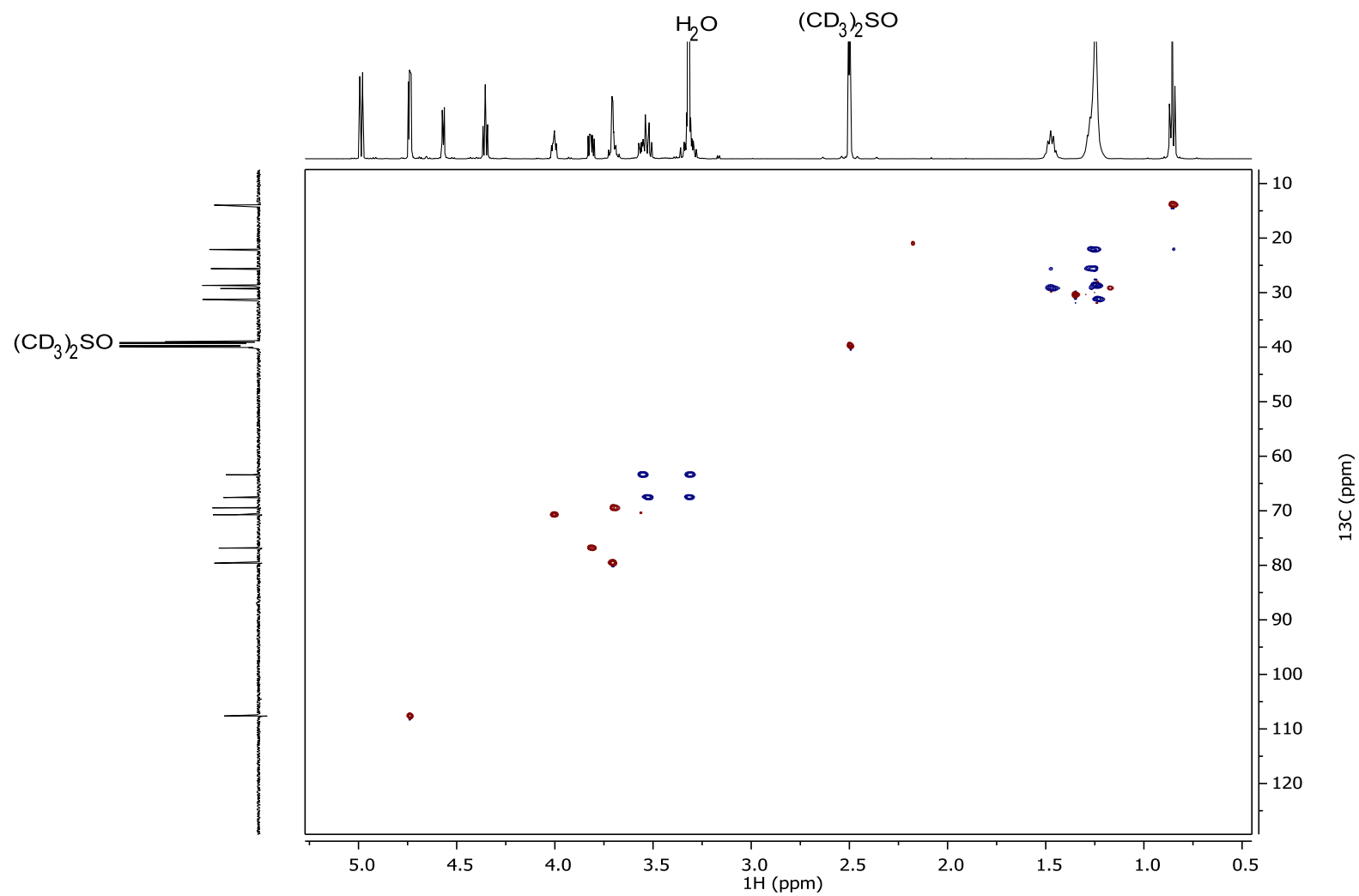
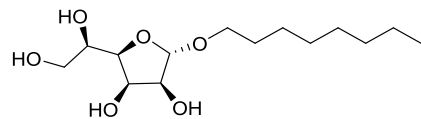
^{13}C NMR (125 MHz, DMSO-d_6) *n*-octyl- α -D-mannofuranoside (3a)



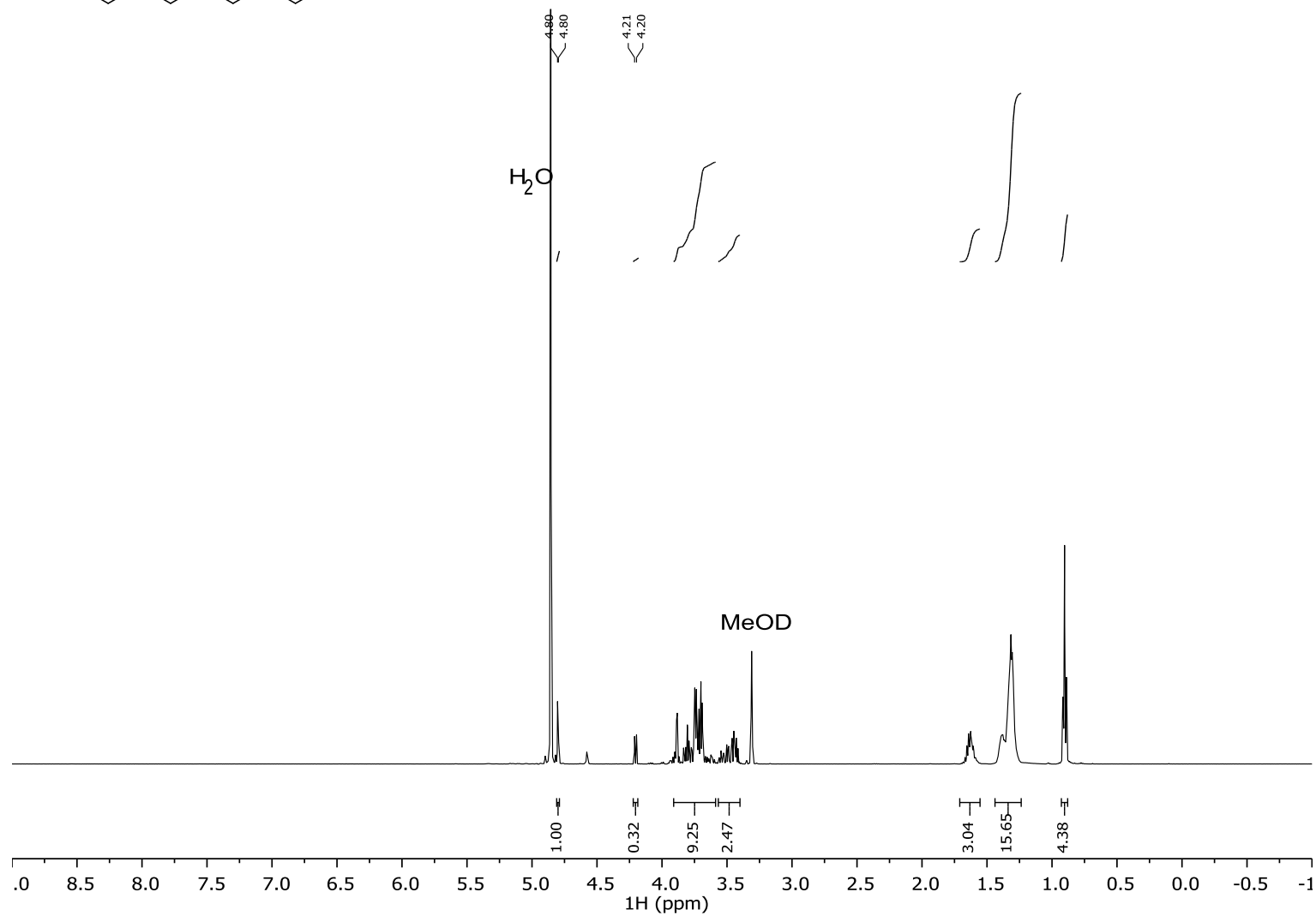
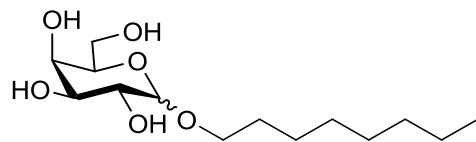
^1H - ^1H COSY NMR (500 MHz, DMSO- d_6) *n*-octyl- α -D-mannofuranoside (3a)



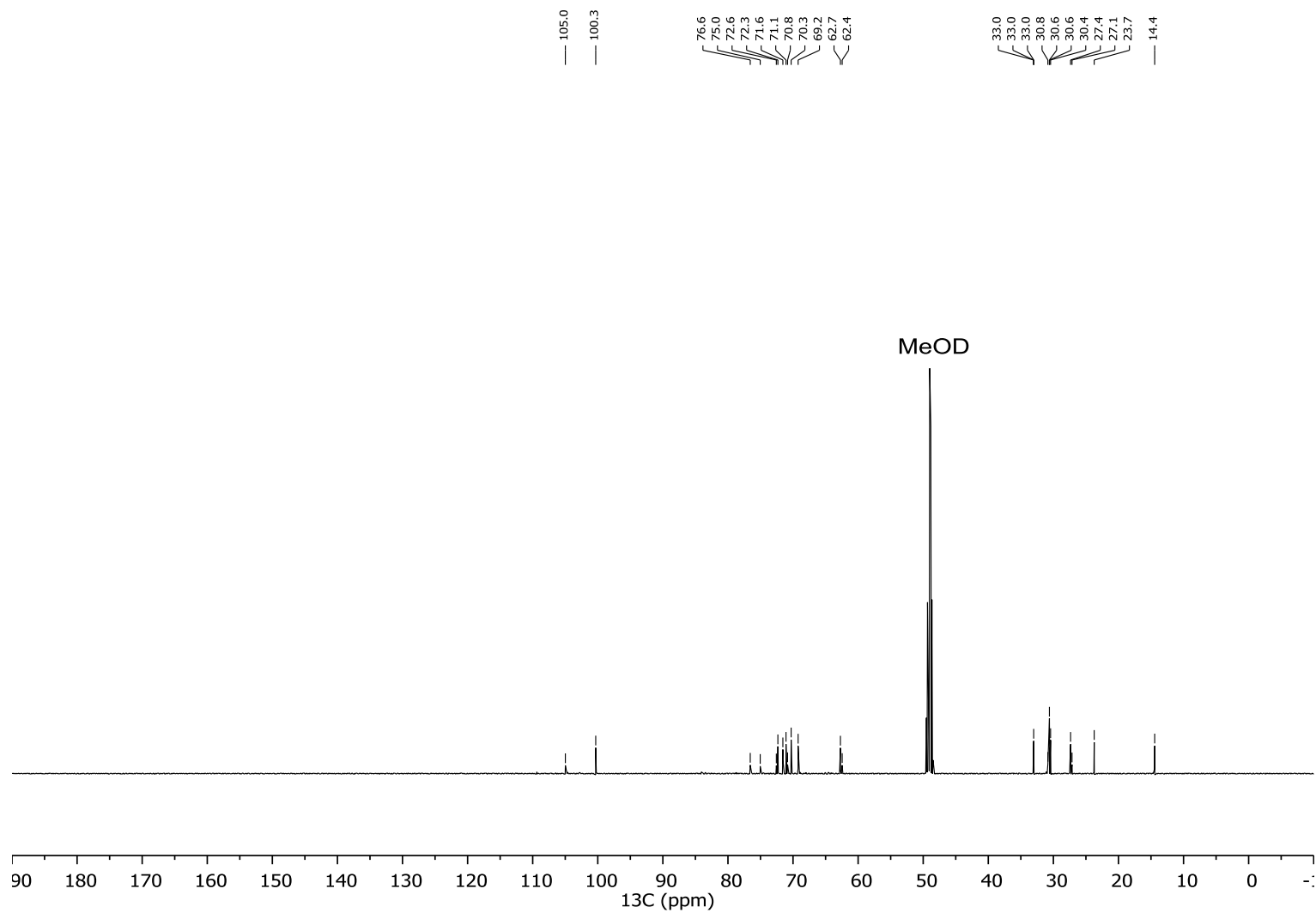
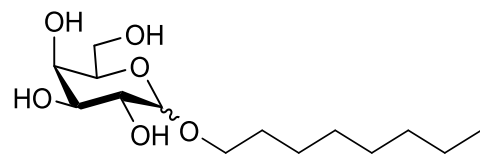
^1H - ^{13}C HSQC NMR (700 MHz, DMSO- d_6) *n*-octyl- α -D-mannofuranoside (3a)



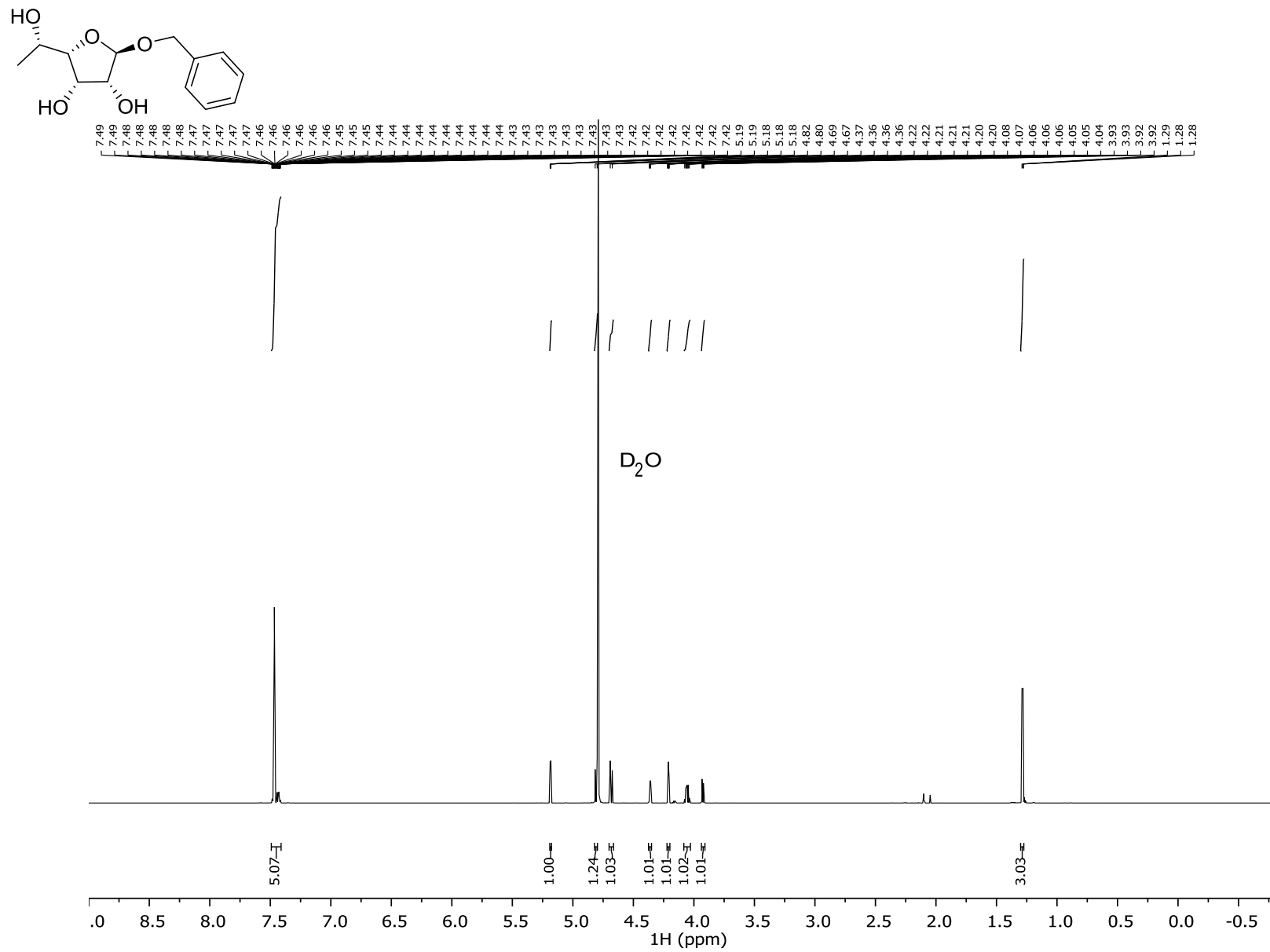
^1H NMR (500 MHz, Methanol- d_4) *n*-octyl-D-galactopyranoside (4a)



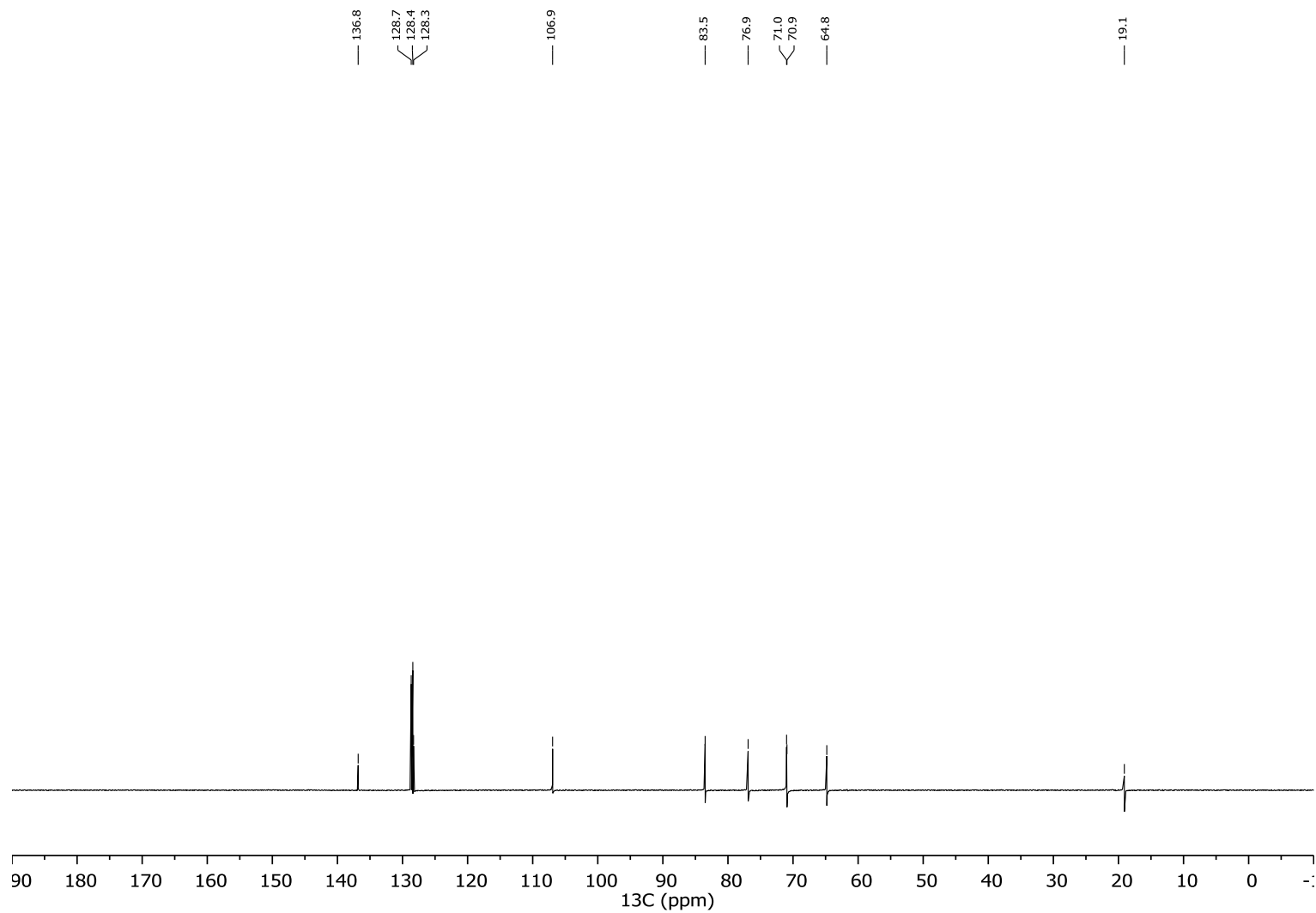
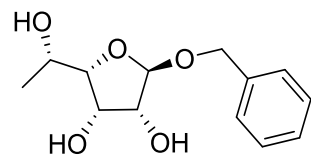
^{13}C NMR (125 MHz, Methanol- d_4) *n*-octyl-D-galactopyranoside (4a)



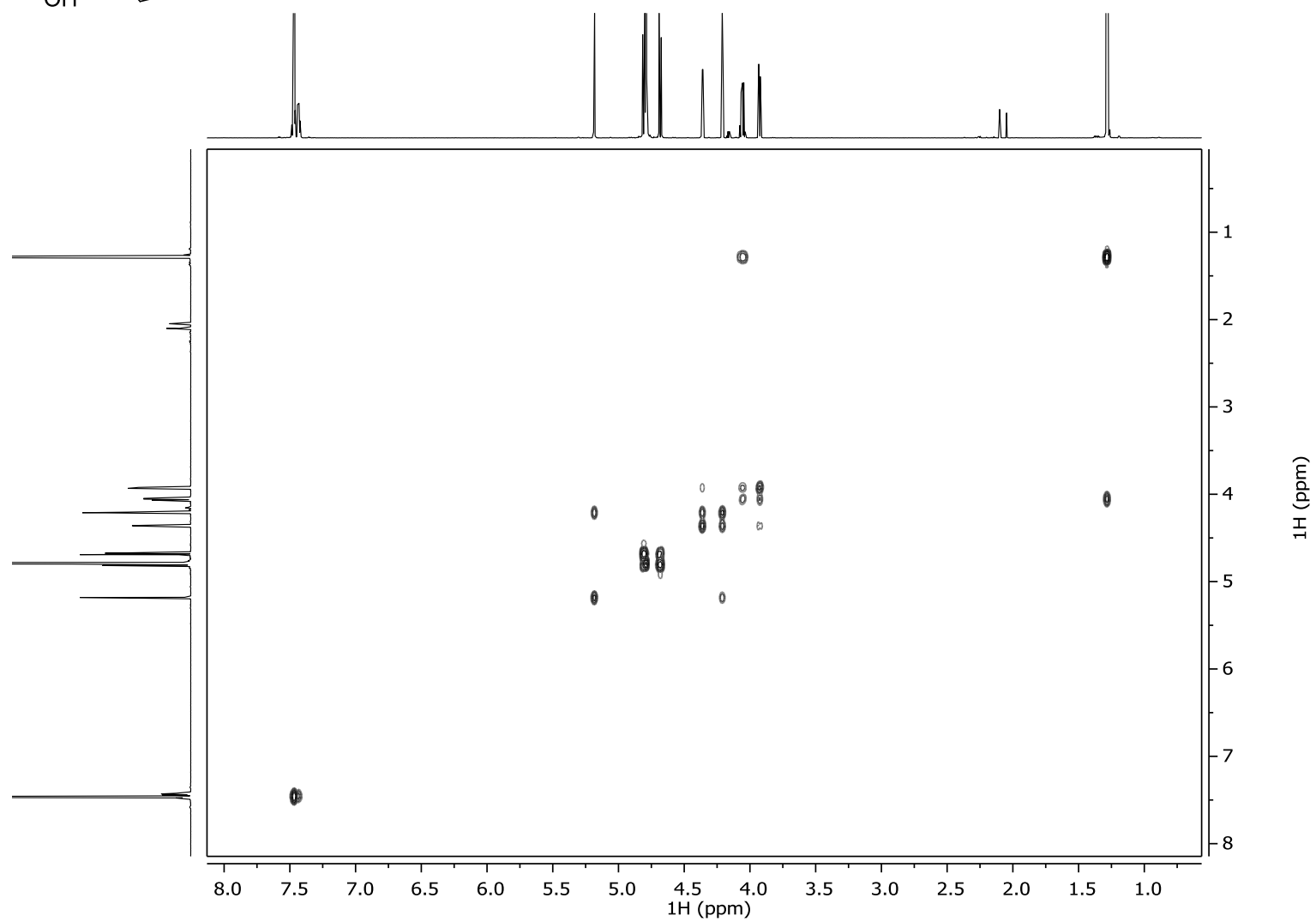
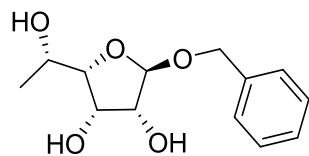
¹H NMR (700 MHz, D₂O) Benzyl α-L-rhamnofuranoside (3c)



^{13}C NMR (125 MHz, D_2O) Benzyl α -L-rhamnofuranoside (3c)

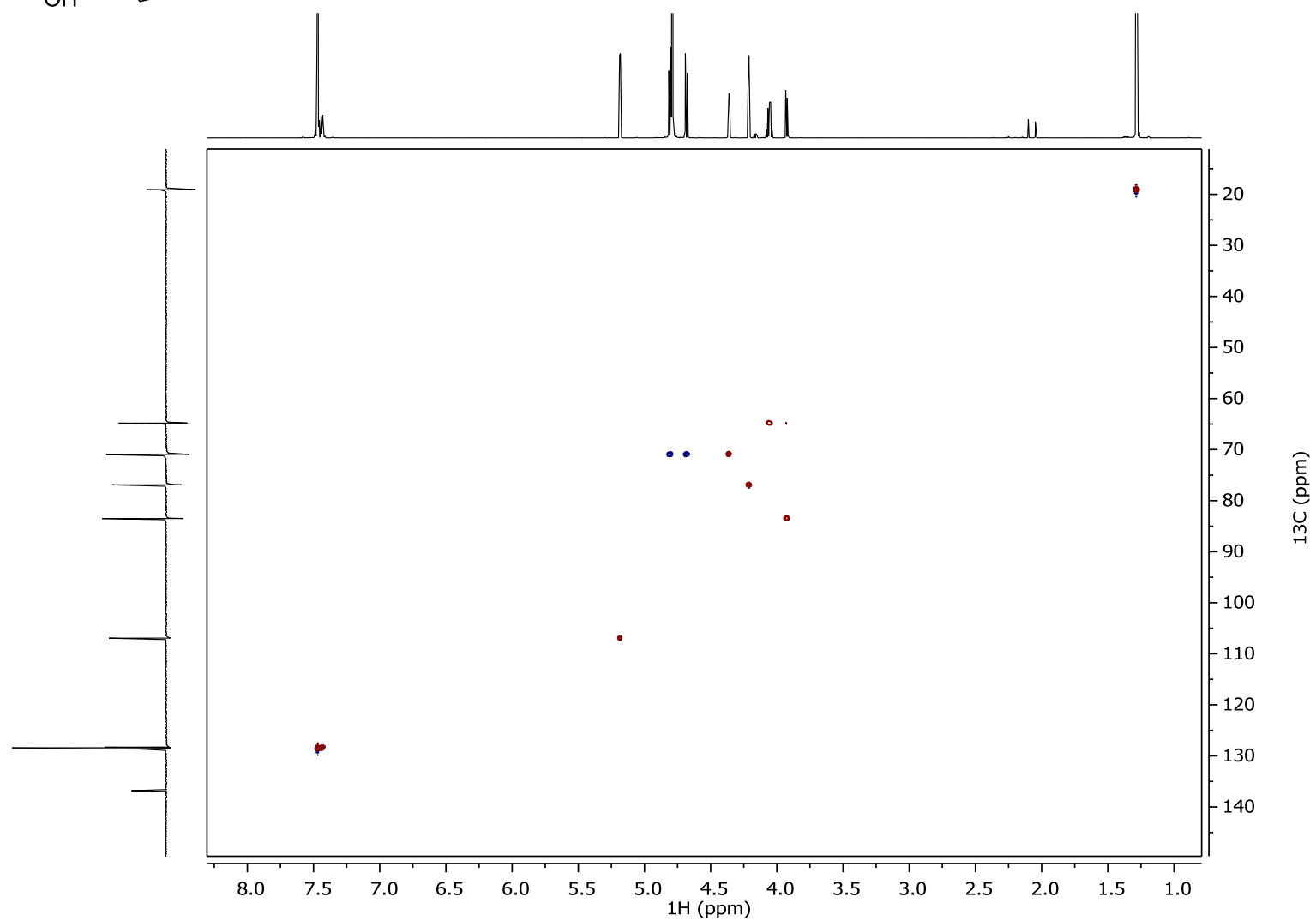
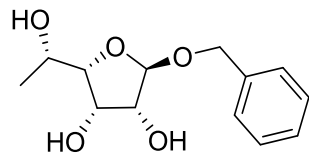


^1H - ^1H COSY NMR (700 MHz, D_2O) Benzyl α -L-rhamnofuranoside (3c)

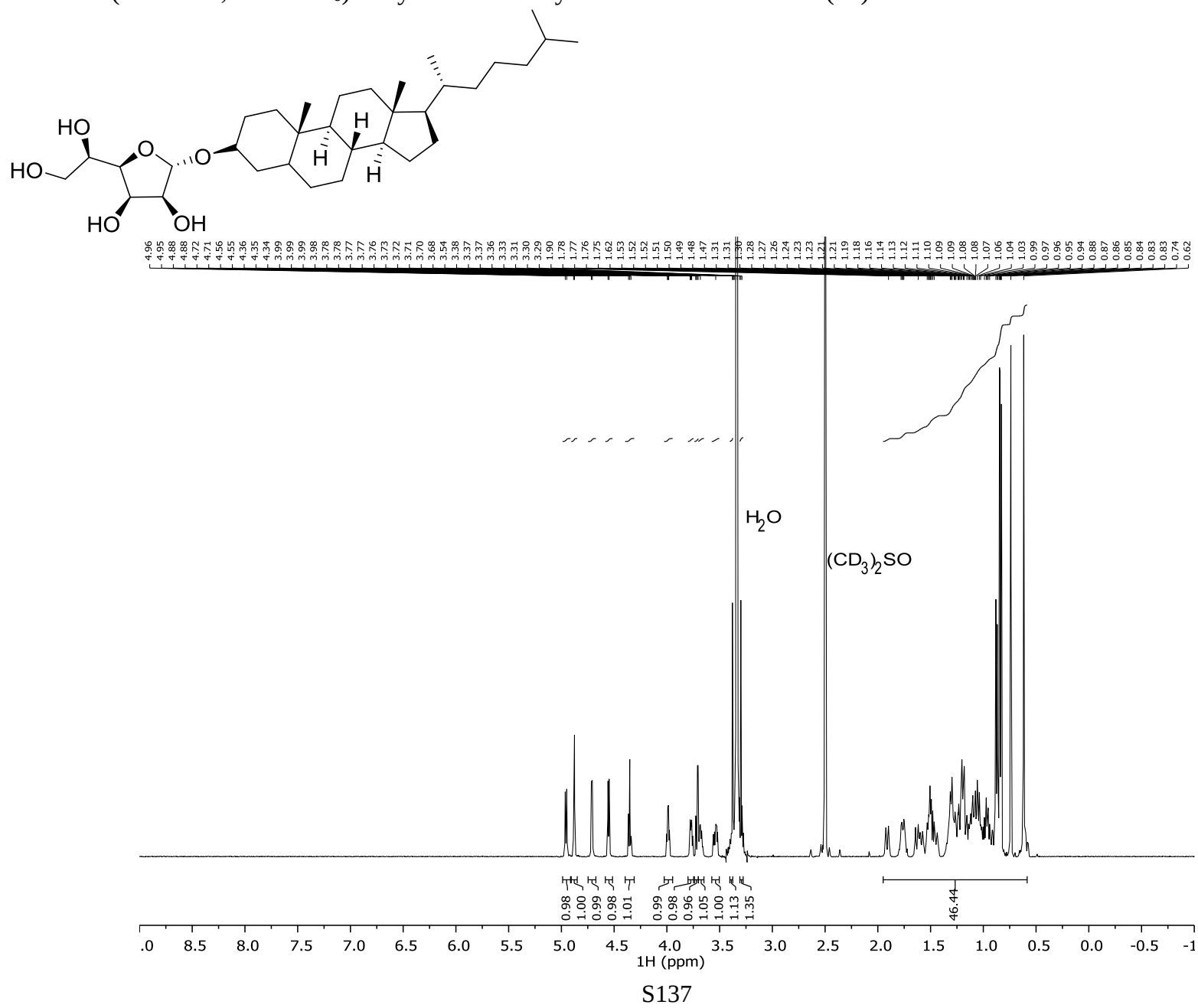


S135

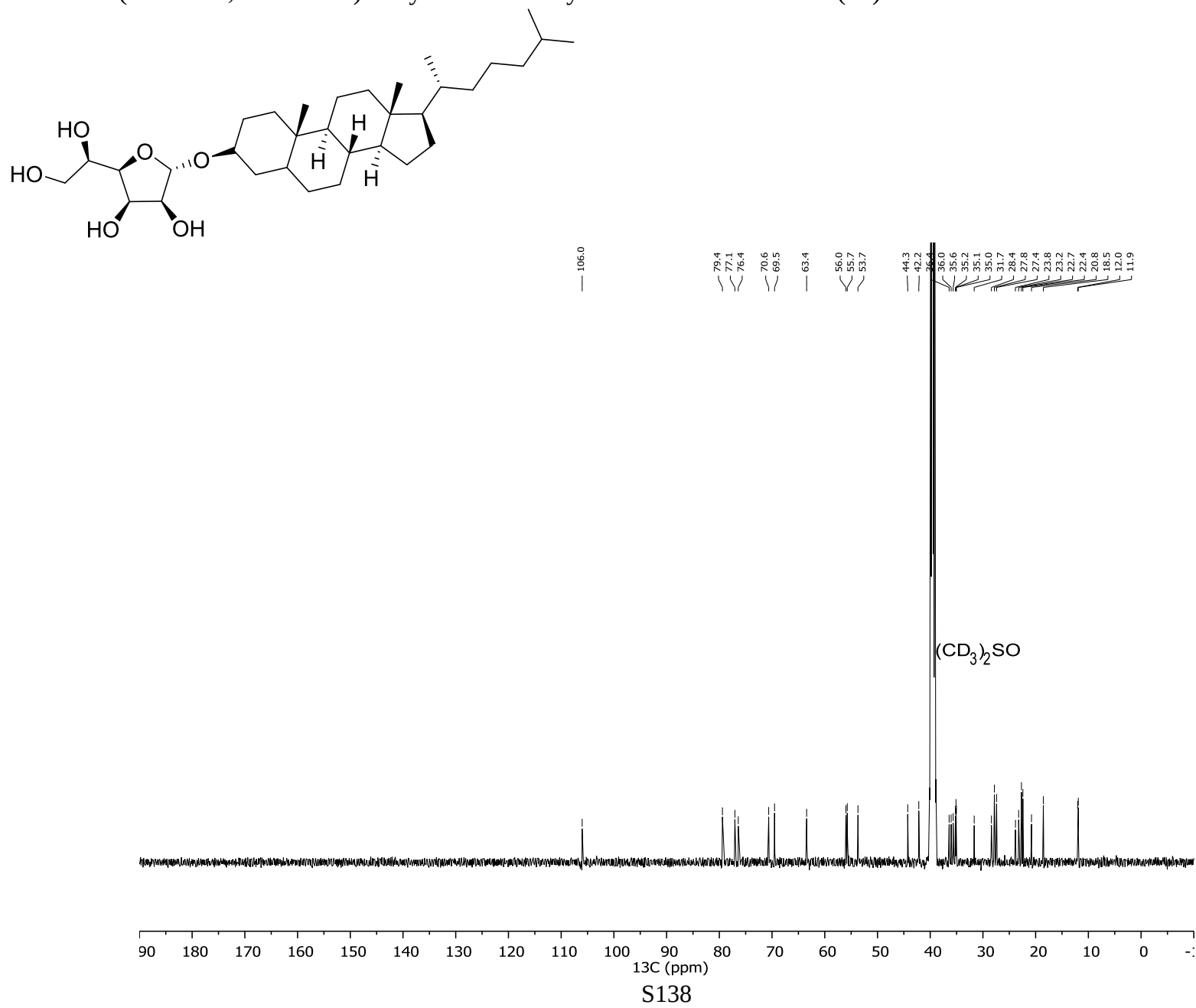
^1H - ^{13}C HSQC NMR (700 MHz, D_2O) Benzyl α -L-rhamnofuranoside (3c)



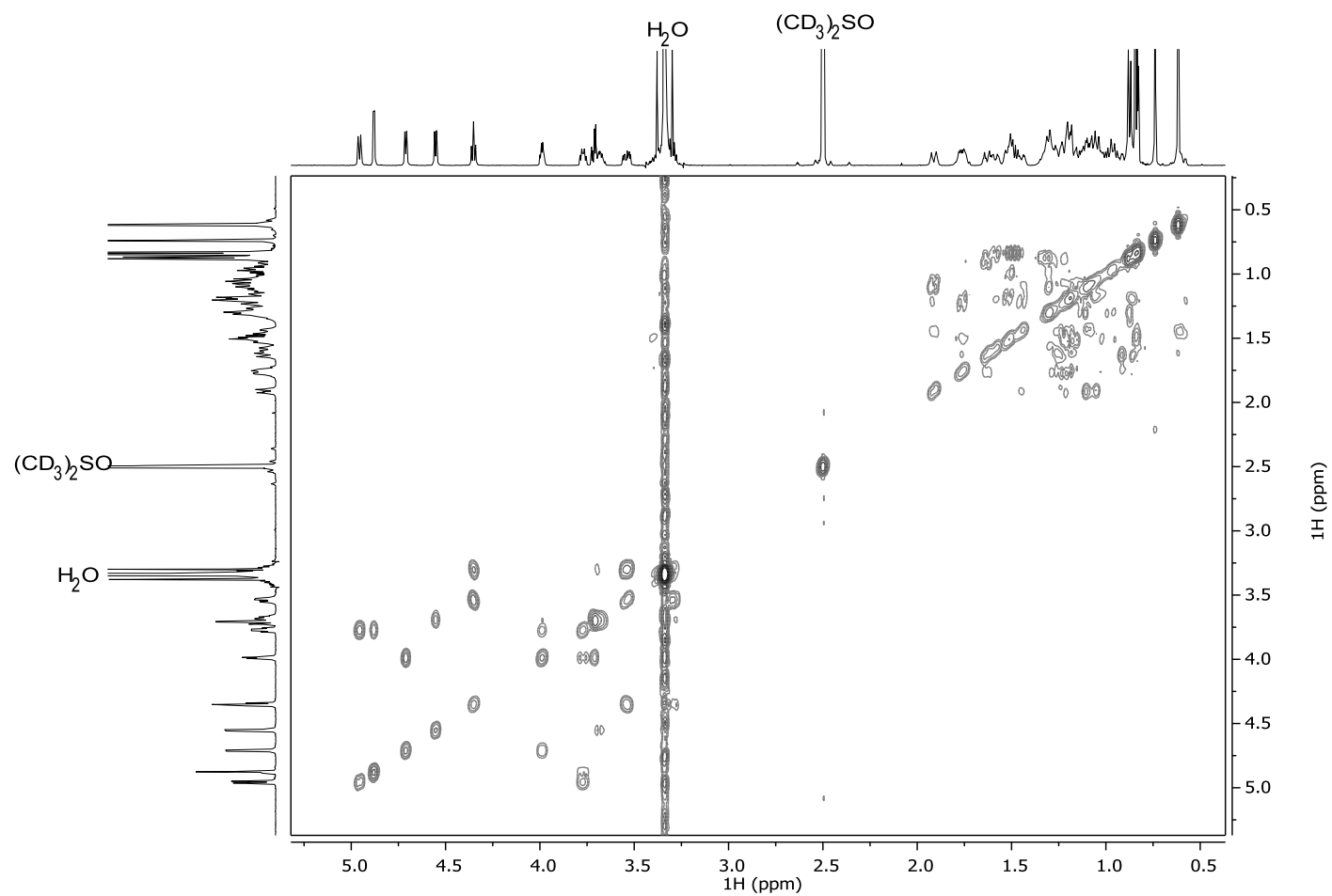
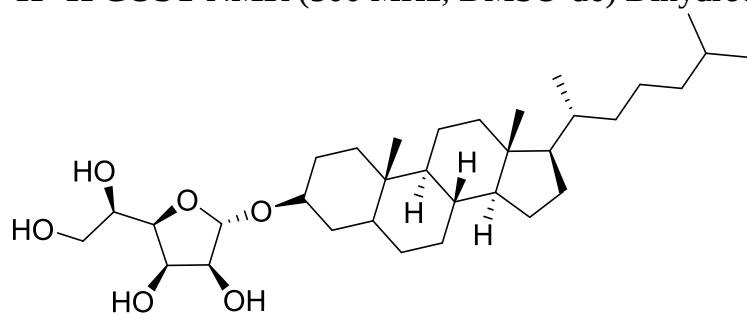
^1H NMR (500 MHz, DMSO-d_6) Dihydrocholesterol- α -D-mannofuranoside (3b)



^{13}C NMR (125 MHz, DMSO- d_6) Dihydrocholesterol- α -D-mannofuranoside (3b)

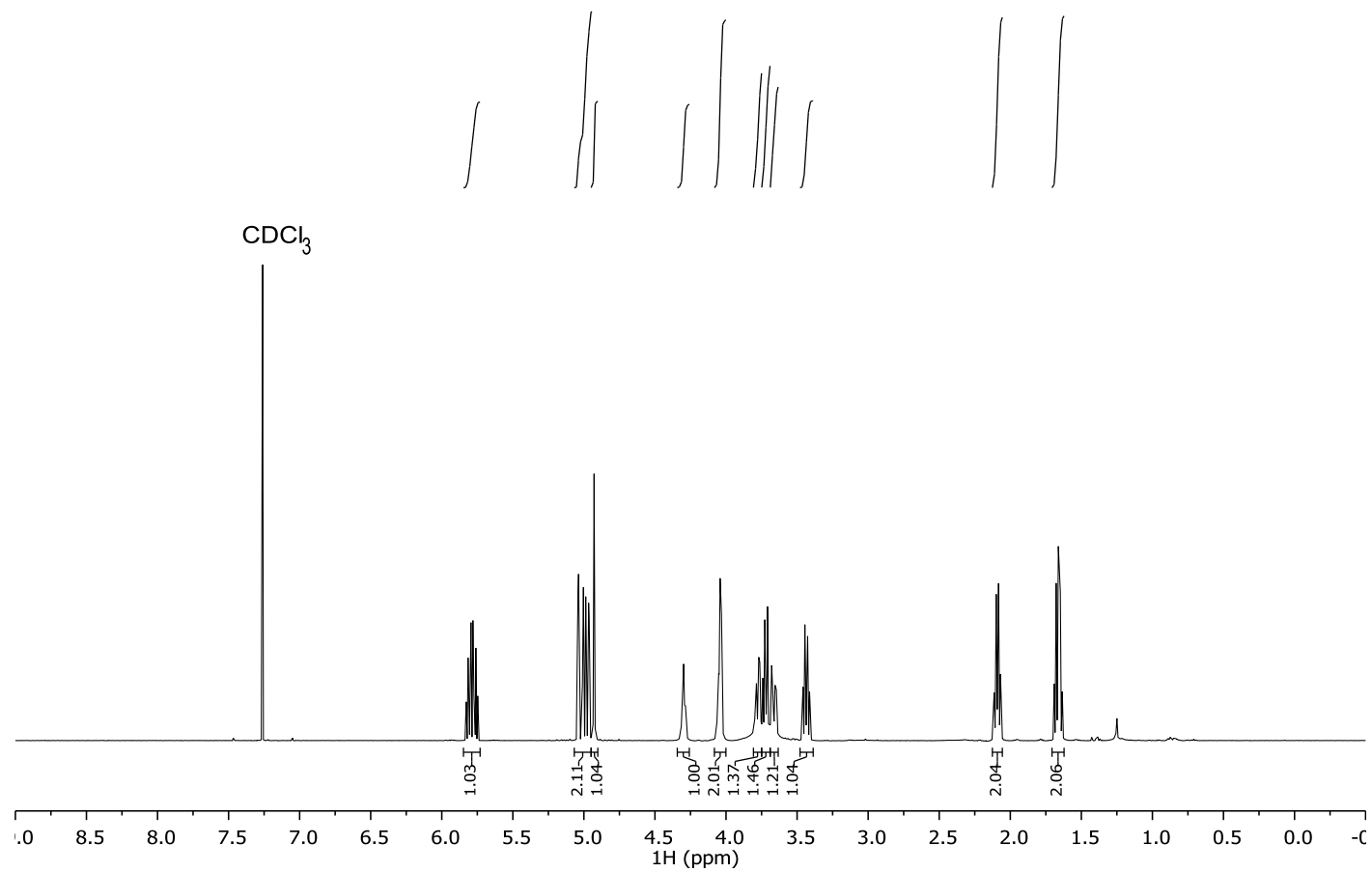
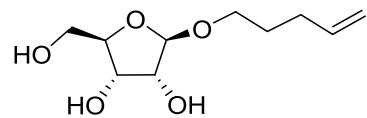


^1H - ^1H COSY NMR (500 MHz, DMSO- d_6) Dihydrocholesterol- α -D-mannofuranoside (3b)

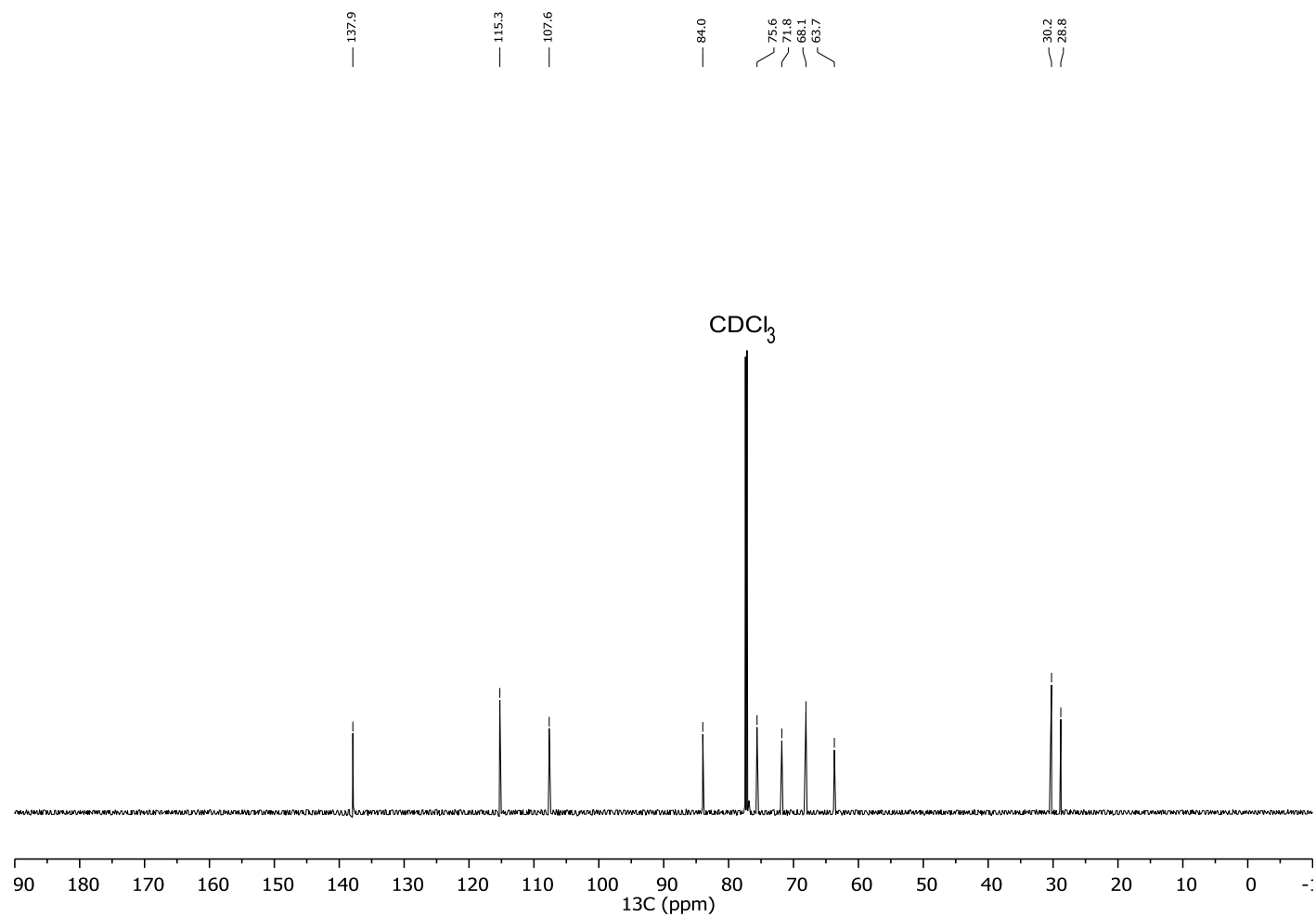
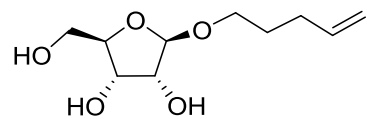


S139

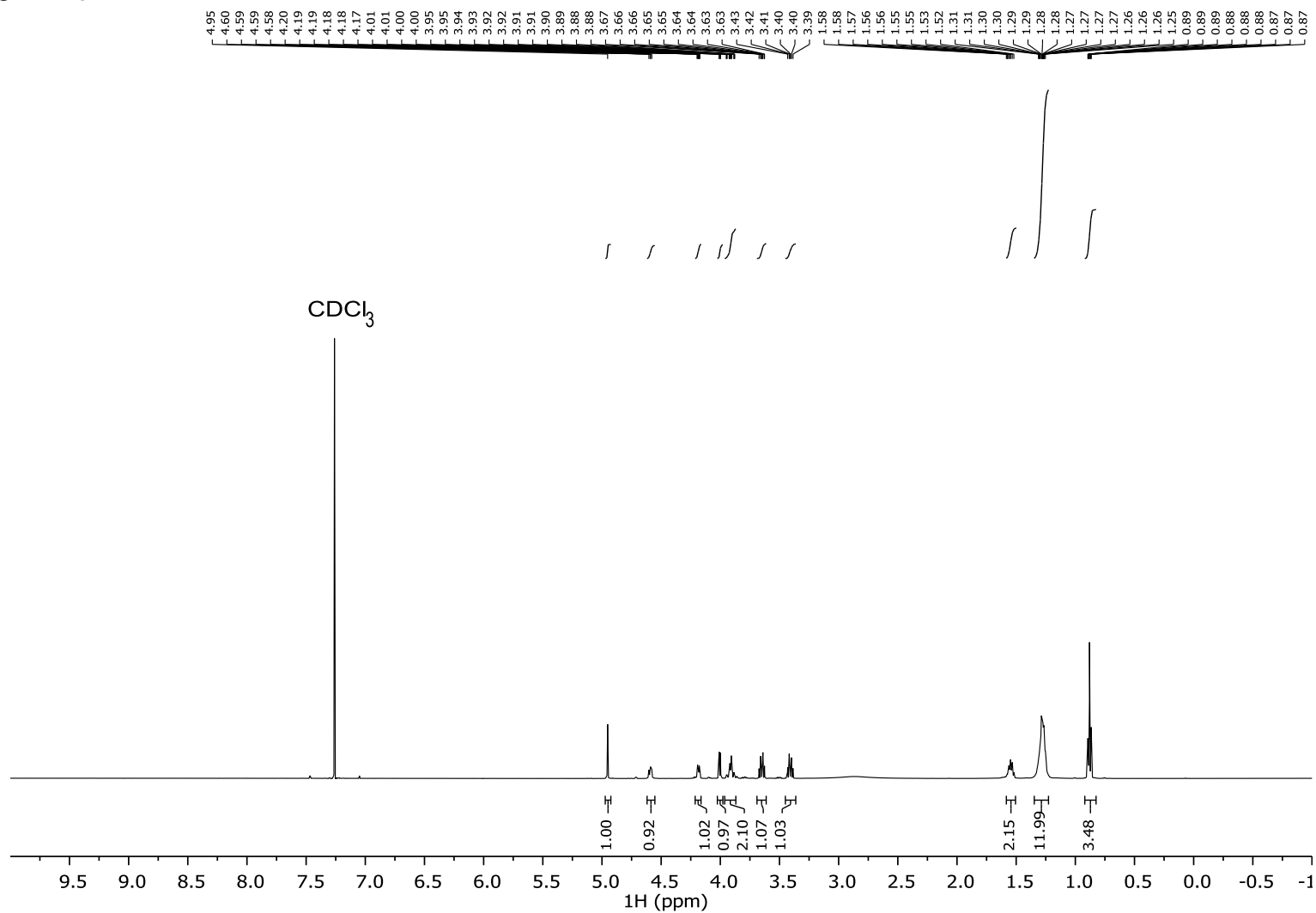
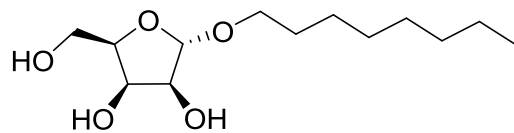
^1H NMR (500 MHz, CDCl_3) *n*-pentenyl- β -D-ribofuranoside (3d)



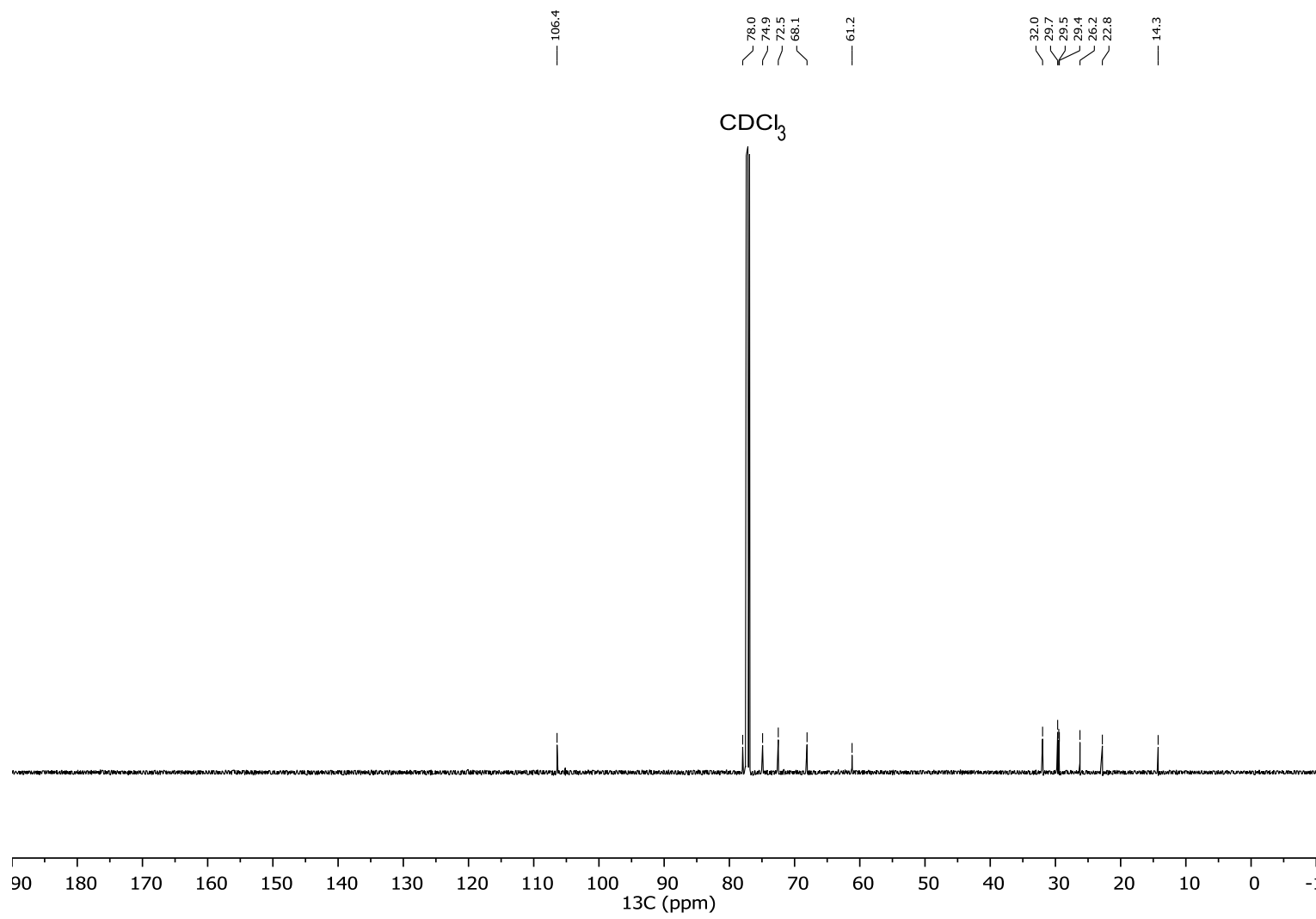
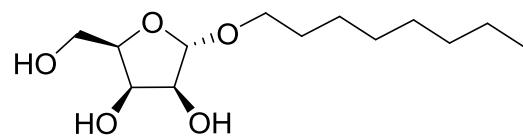
^{13}C NMR (126 MHz, CDCl_3) *n*-pentenyl- β -D-ribofuranoside (3d)



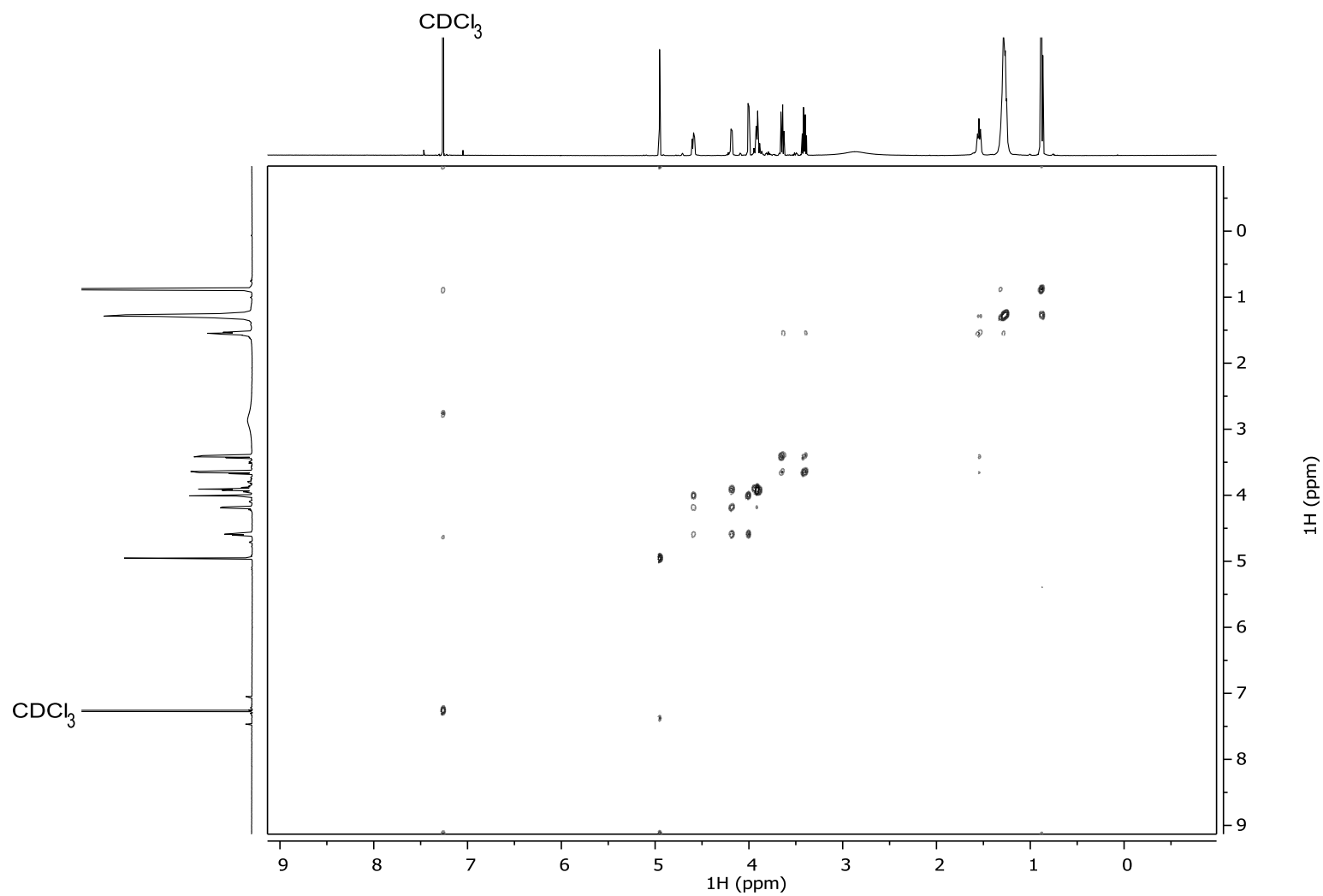
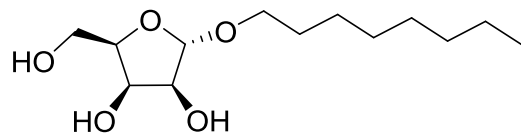
¹H NMR (700 MHz, CDCl₃) *n*-octyl- α -D-lyxofuranoside (3e)



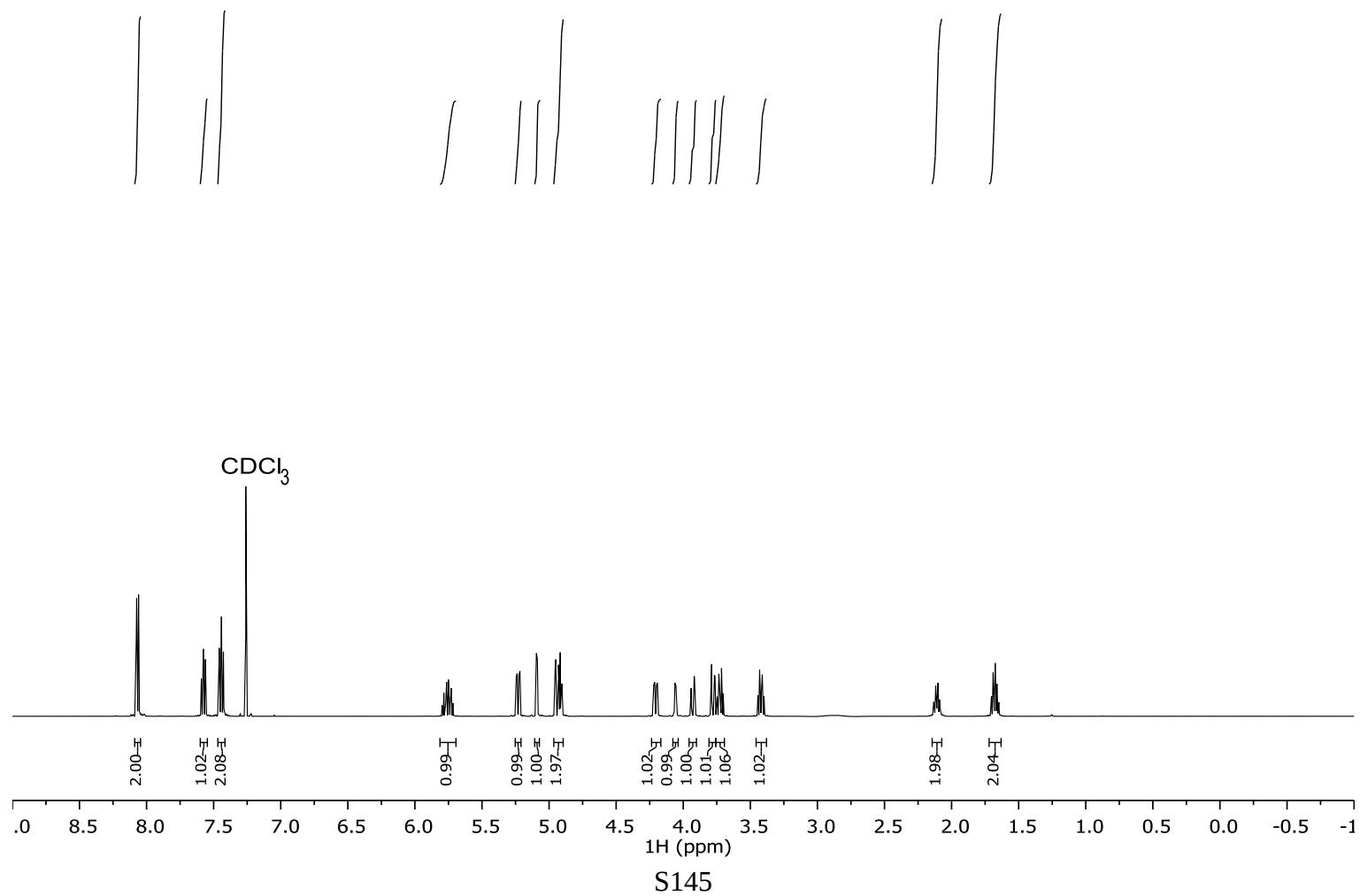
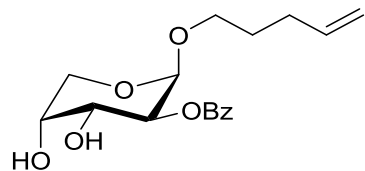
^{13}C NMR (125 MHz, CDCl_3) *n*-octyl- α -D-lyxofuranoside (3e)



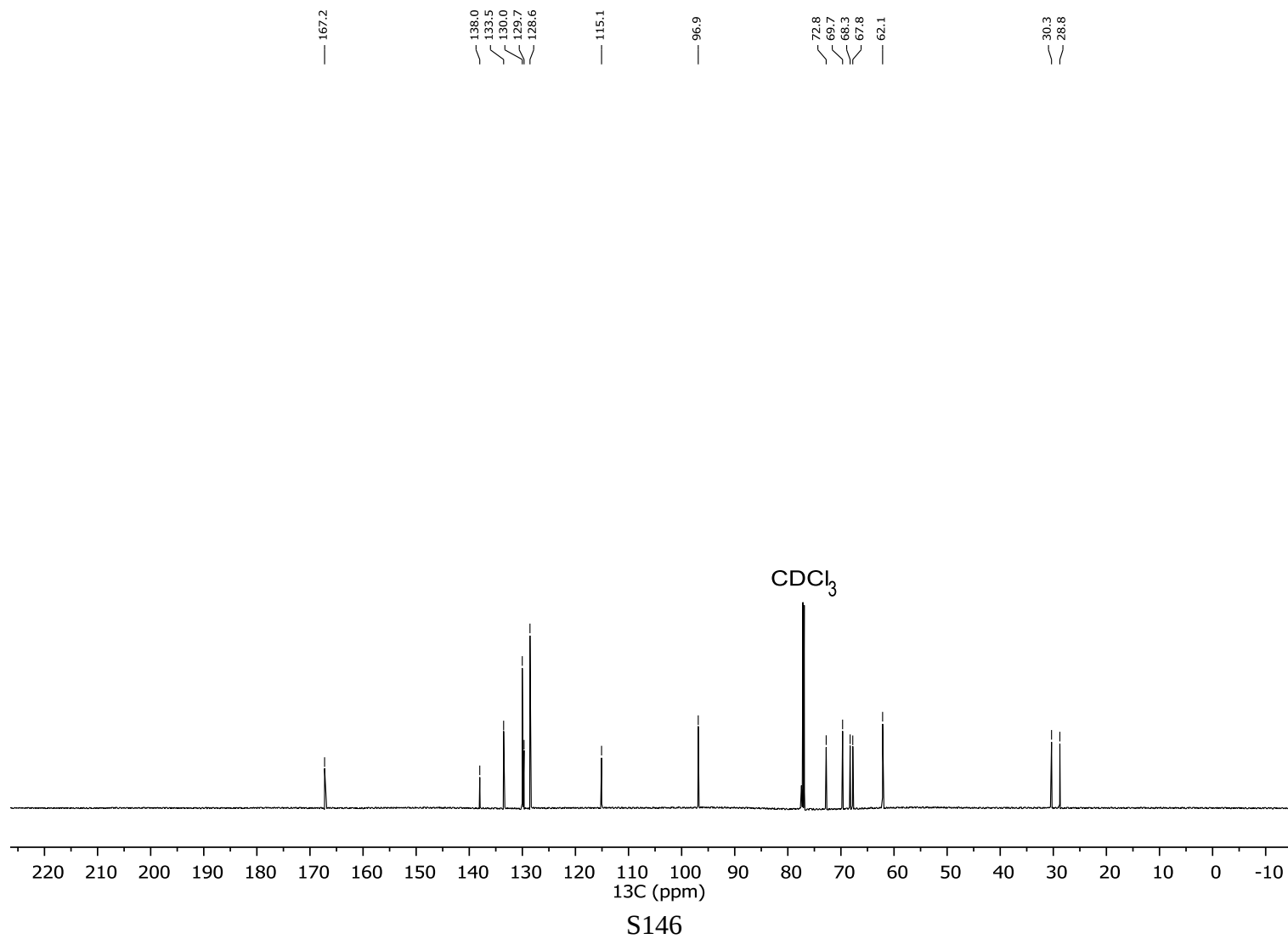
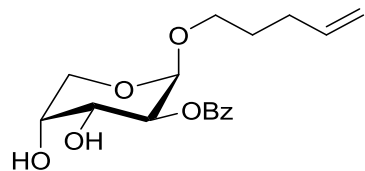
^1H - ^1H COSY NMR (700MHz, CDCl_3) *n*-octyl- α -D-lyxofuranoside (3e)



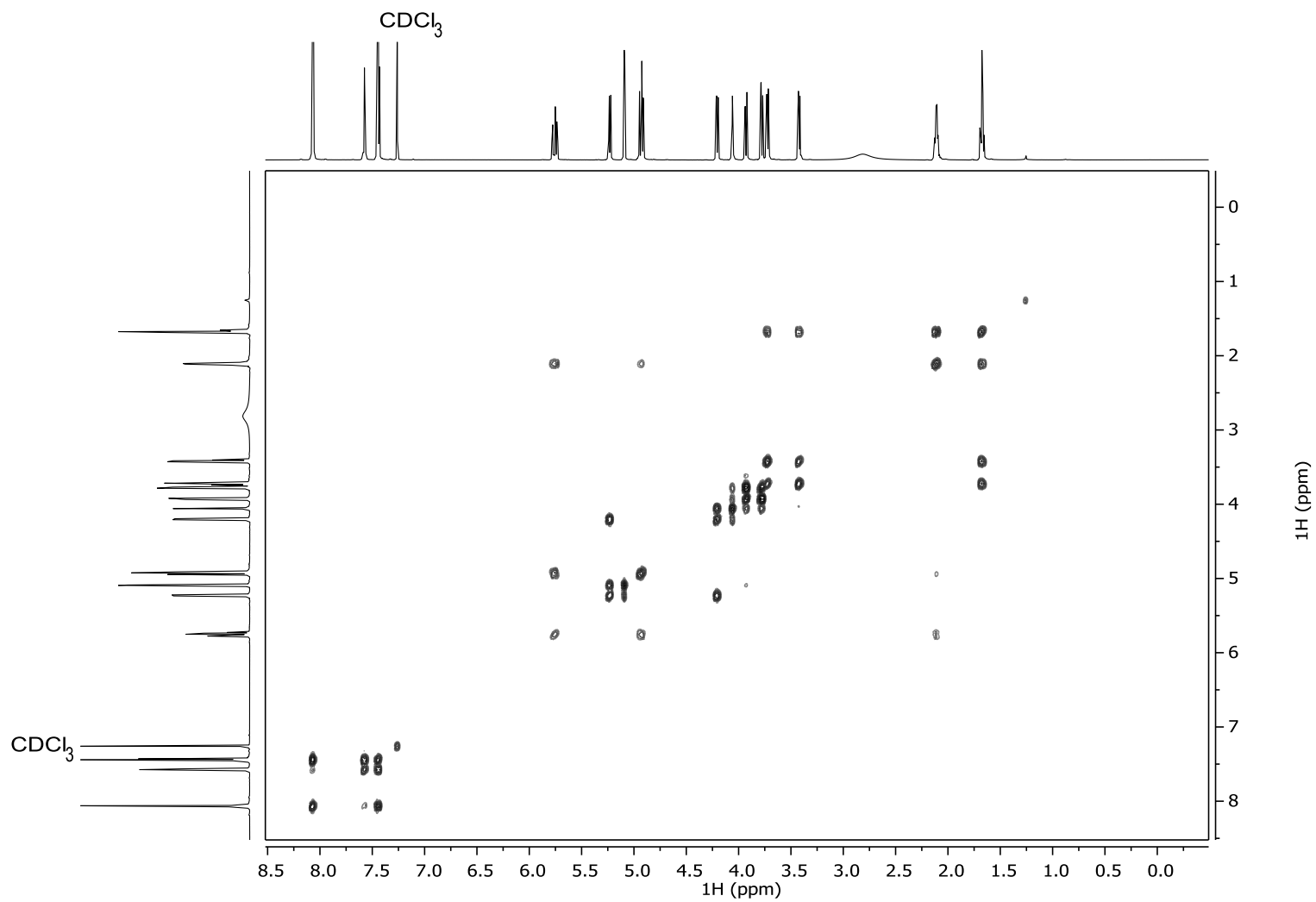
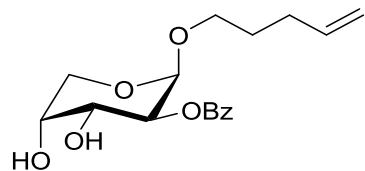
^1H NMR (500 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- β -D-arabinopyranoside (β -6d)



^{13}C NMR (126 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- β -D-arabinopyranoside (β -6d)

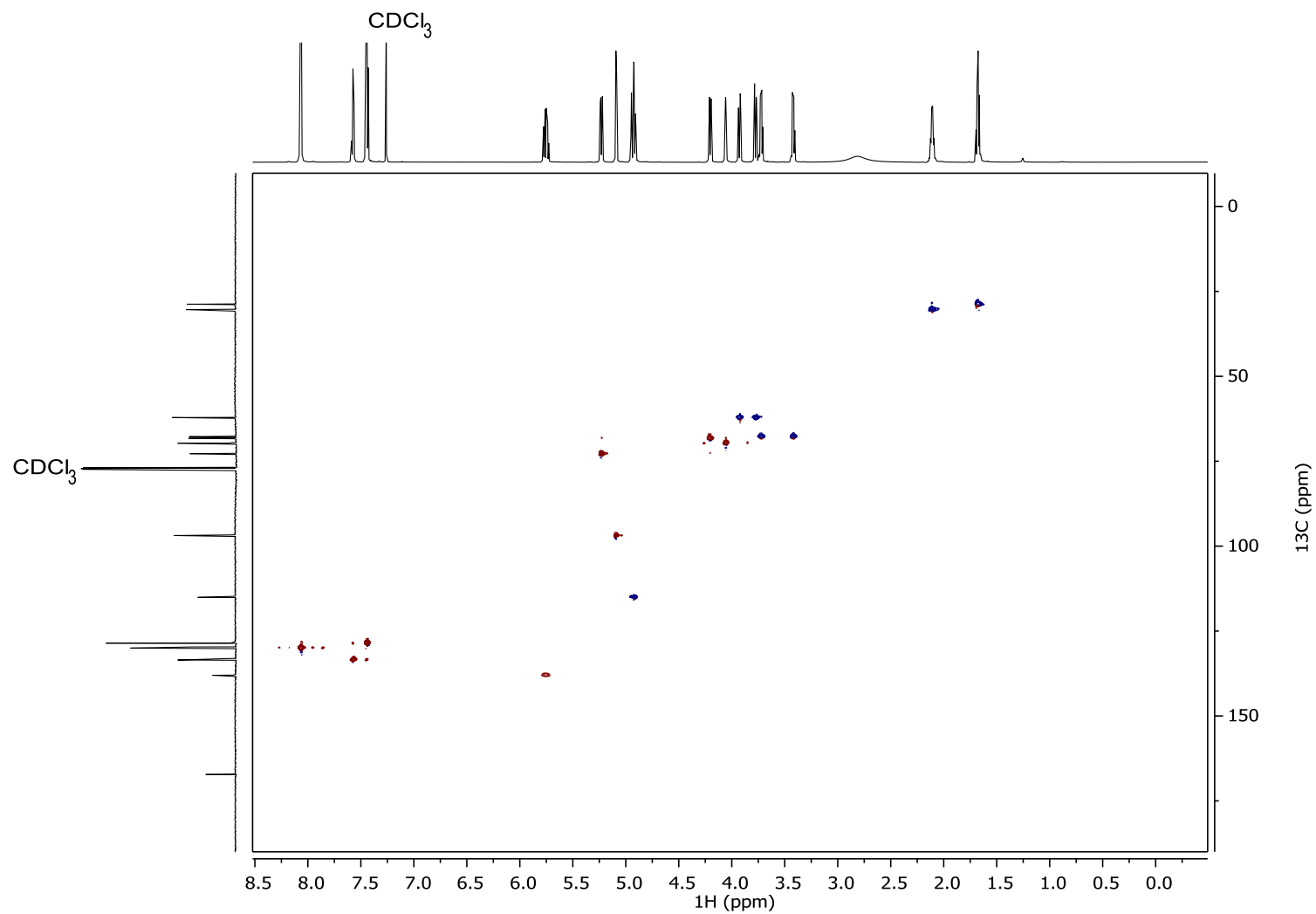
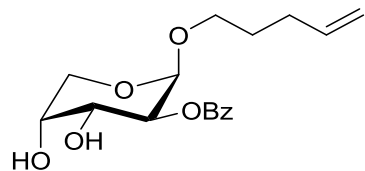


^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- β -D-arabinopyranoside (β -6d)



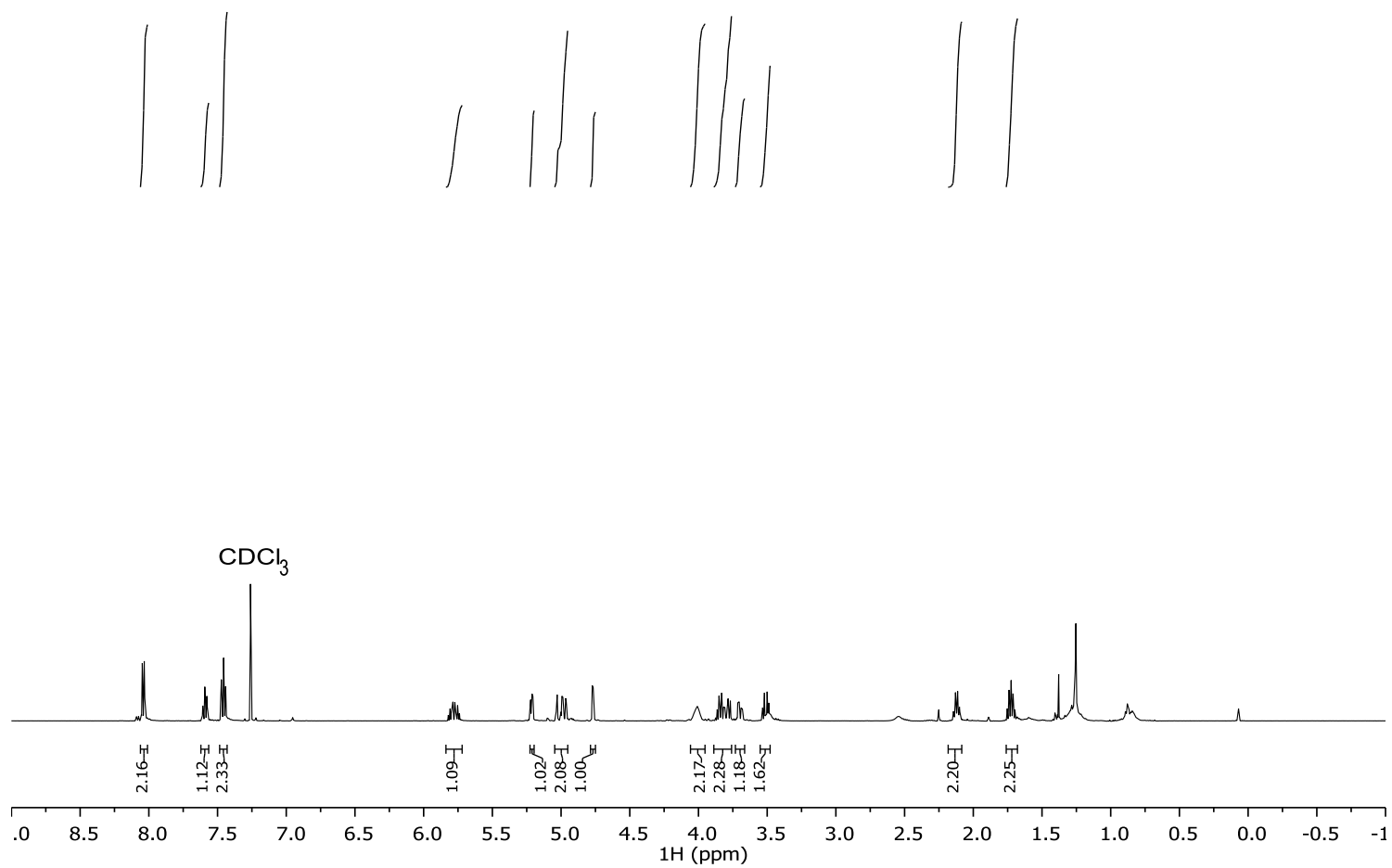
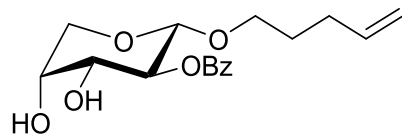
S147

^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- β -D-arabinopyranoside (β -6d)

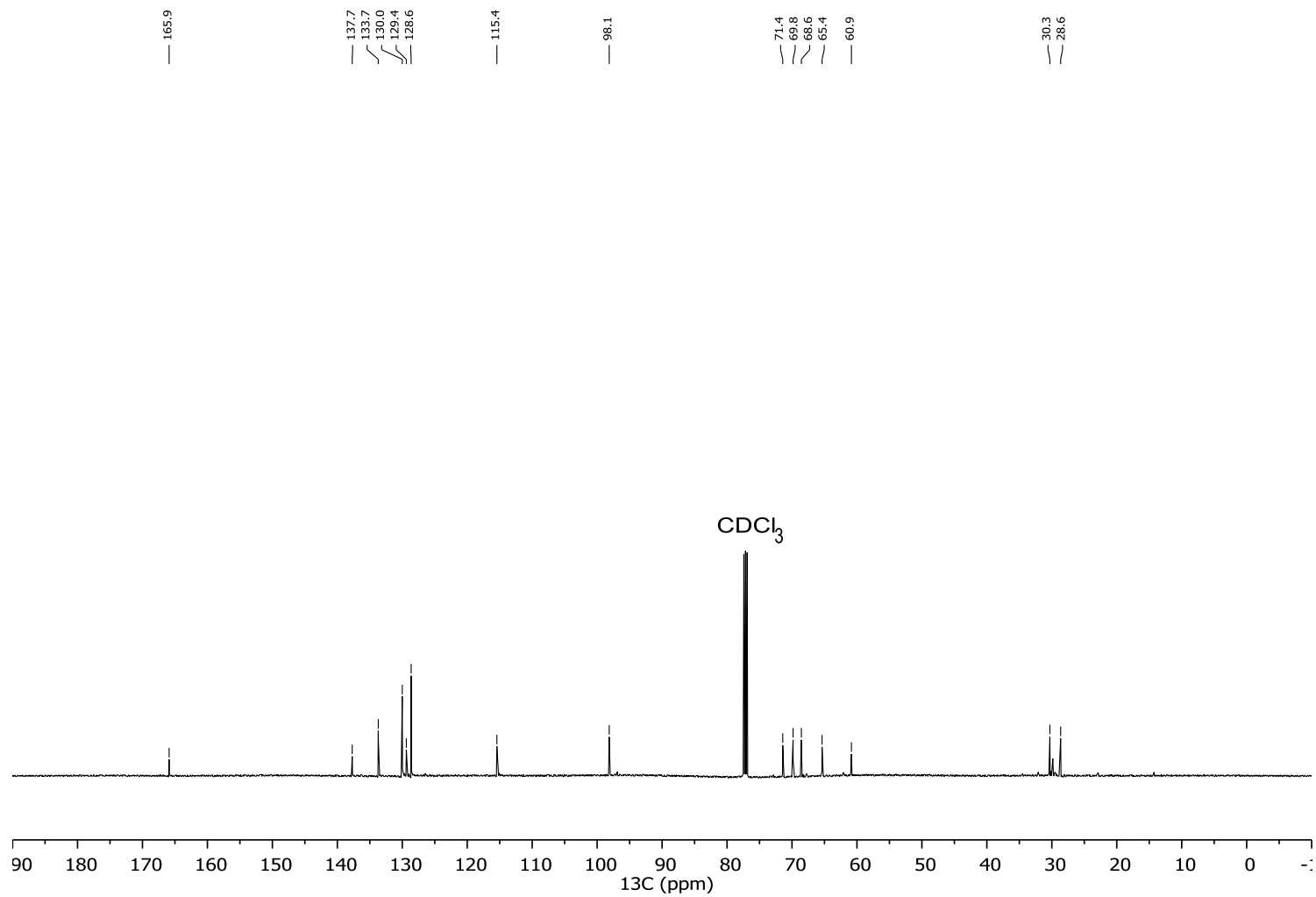
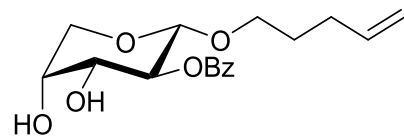


S148

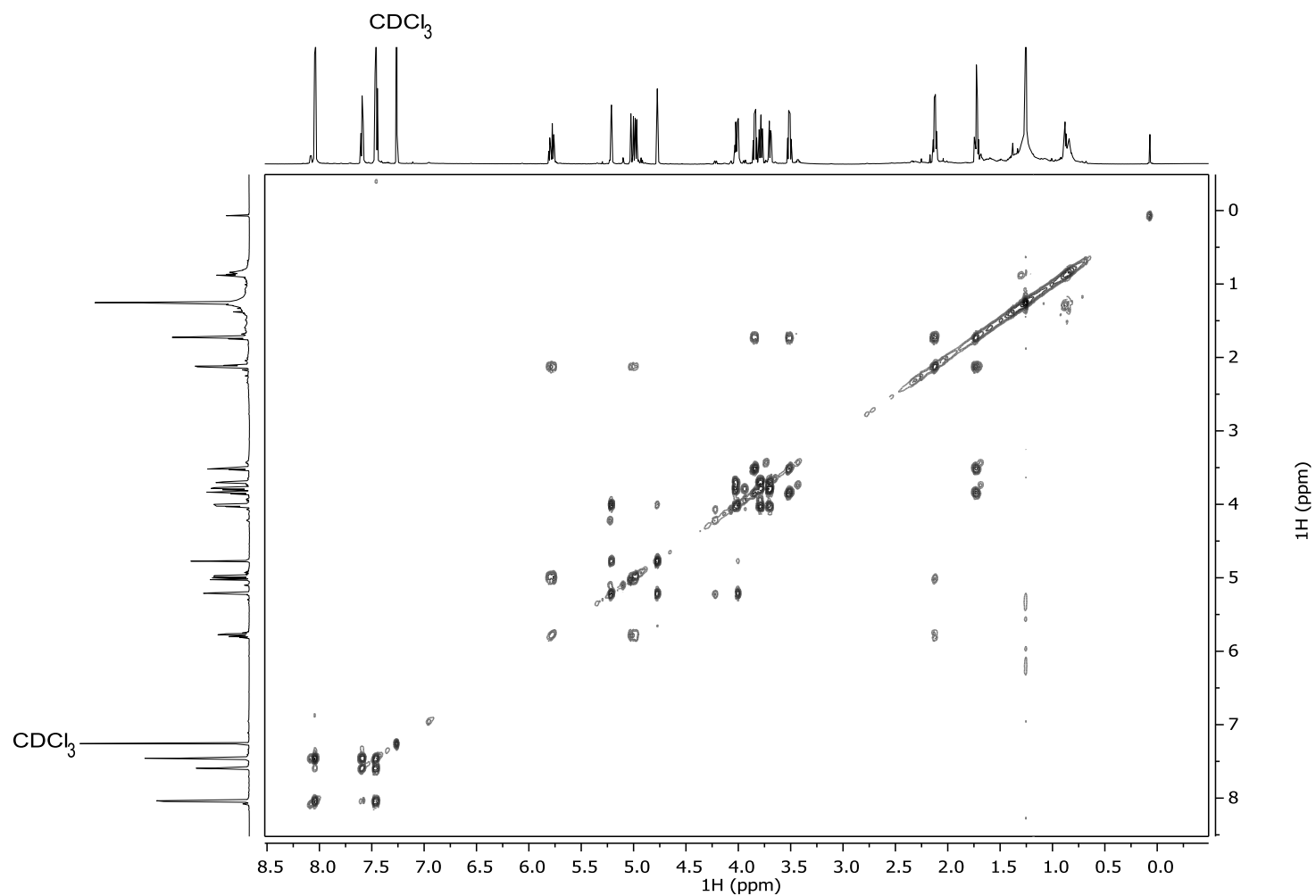
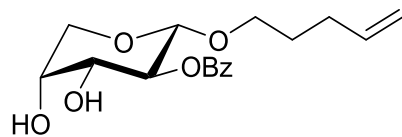
^1H NMR (500 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- α -D-arabinopyranoside (α -6d)



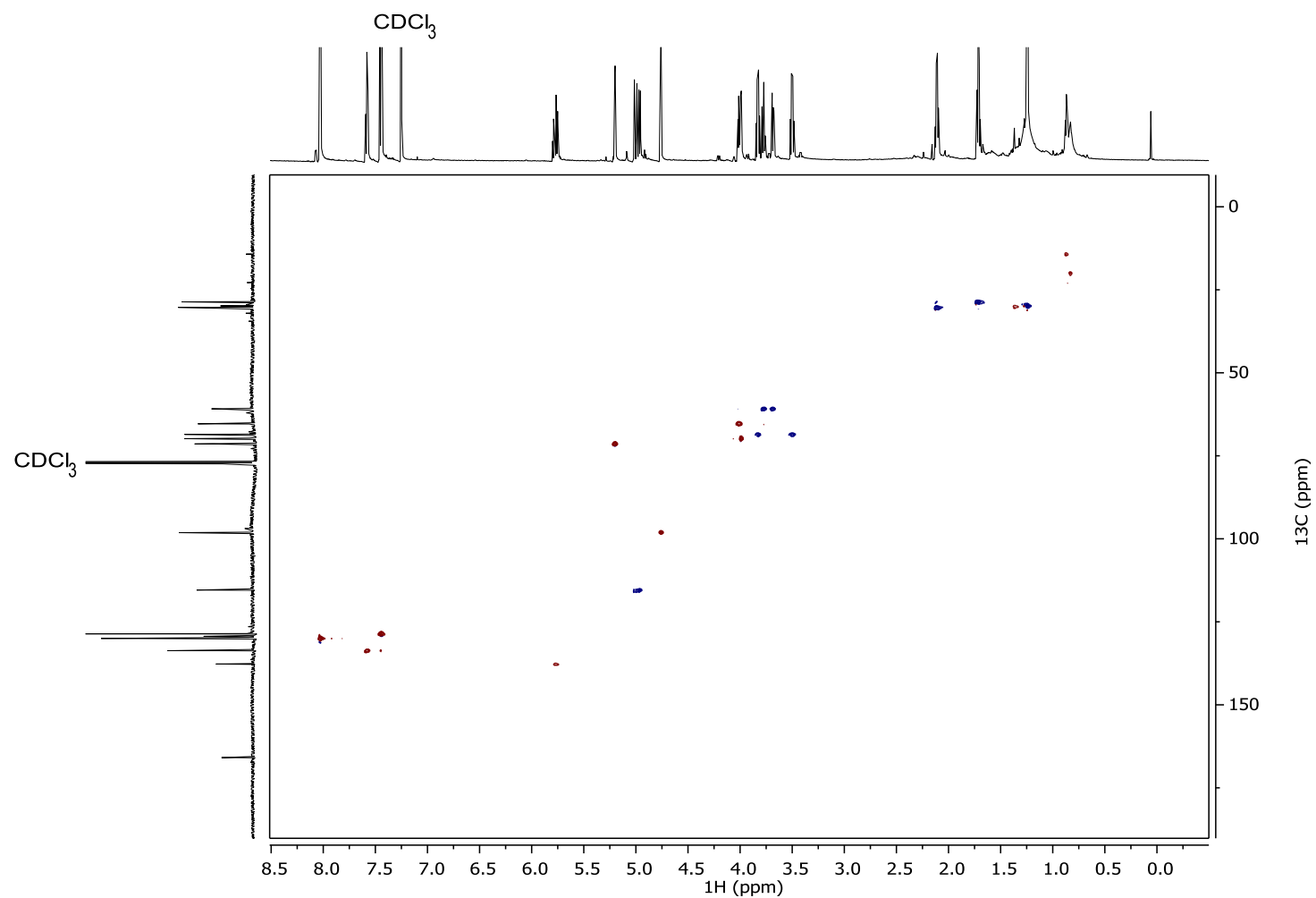
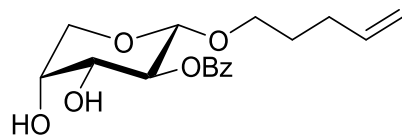
^{13}C NMR (126 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- α -D-arabinopyranoside (α -6d)



^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- α -D-arabinopyranoside (α -6d)

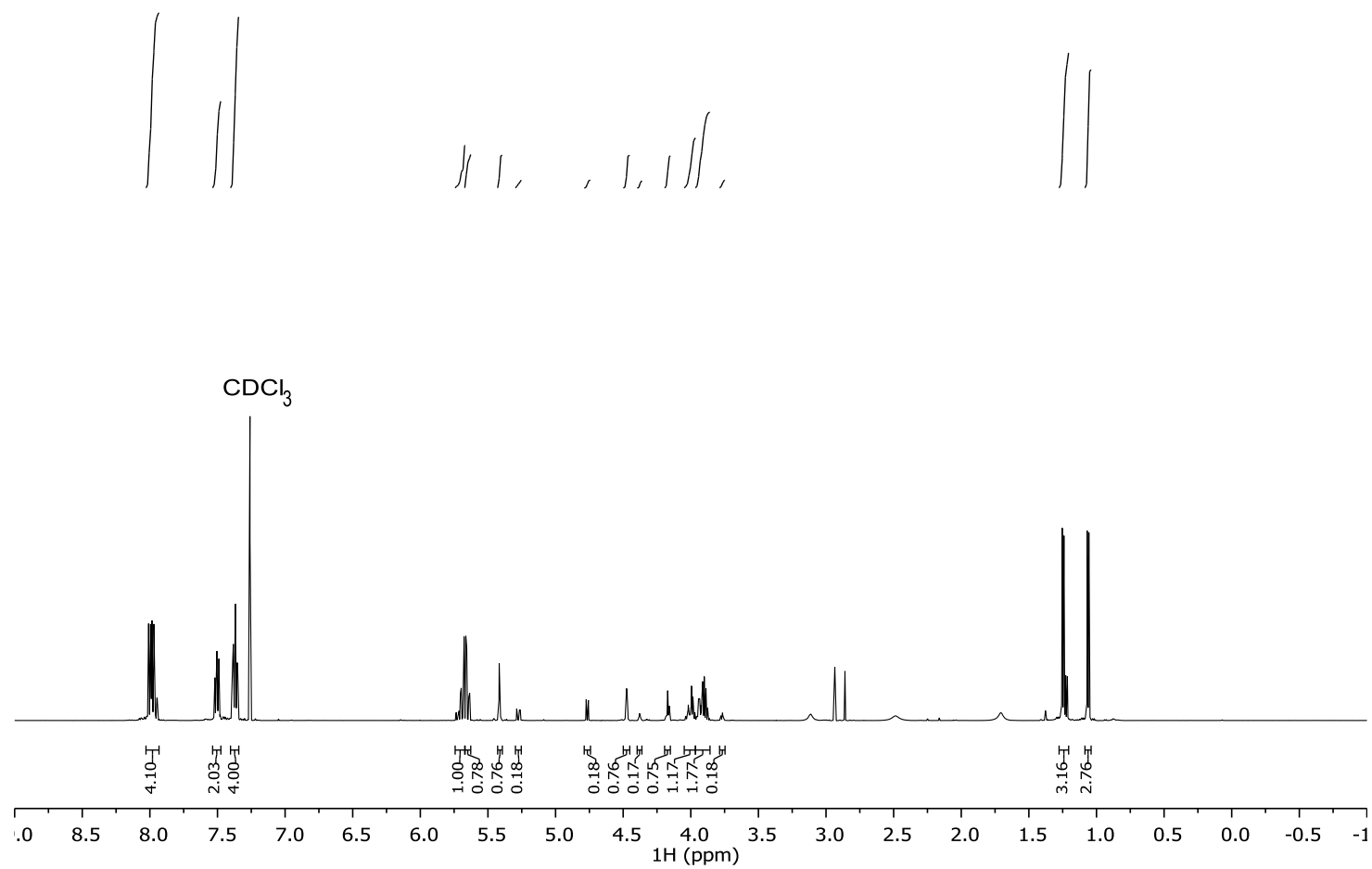
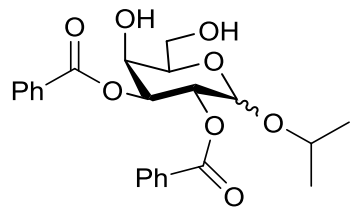


^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-pentenyl 2-*O*-benzoyl- α -D-arabinopyranoside (α -6d)

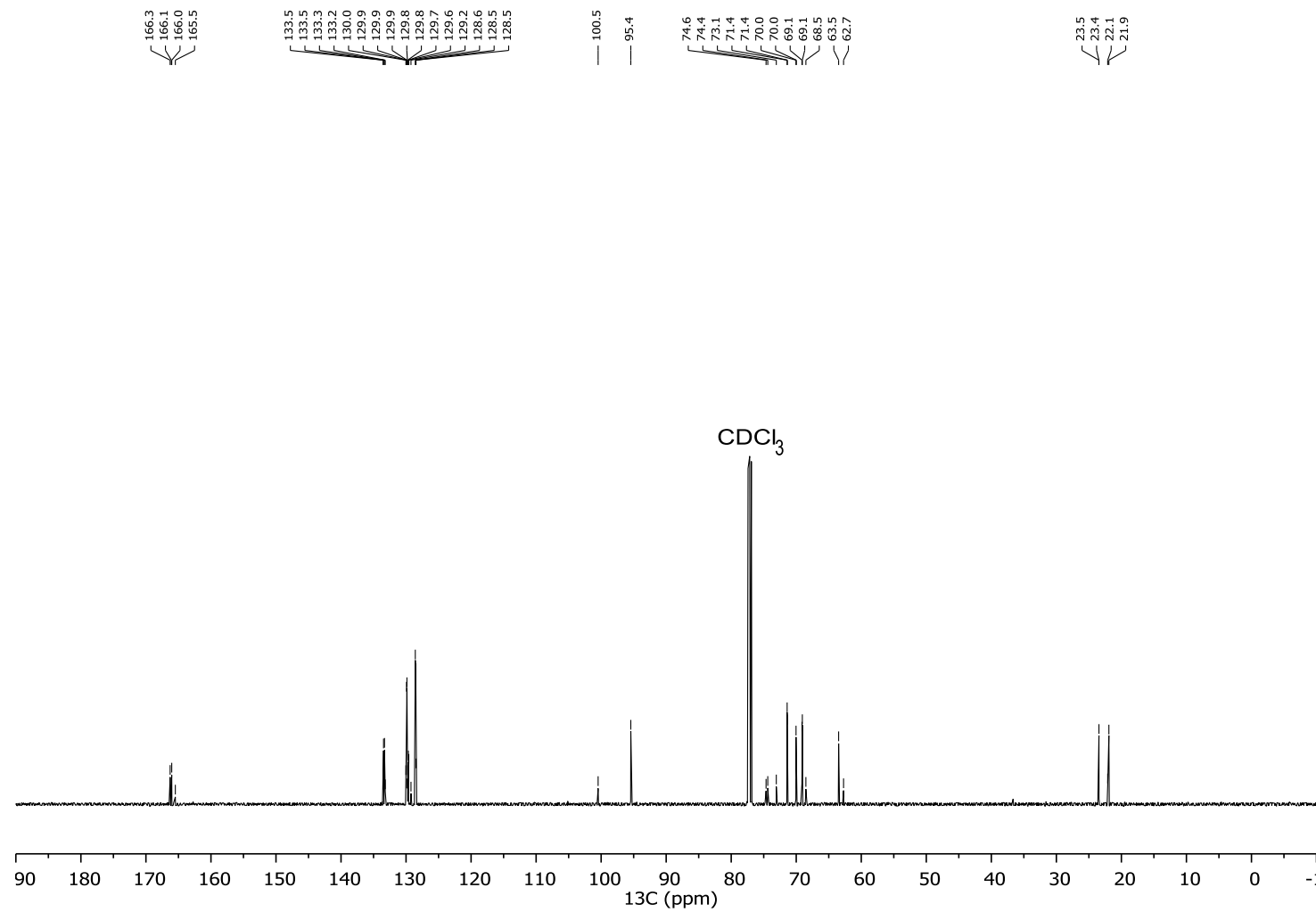
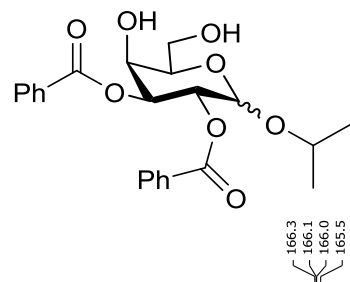


¹H NMR (500 MHz, CDCl₃) Isopropyl 2,3-di-O-benzoyl-D-galactopyranoside (6a)

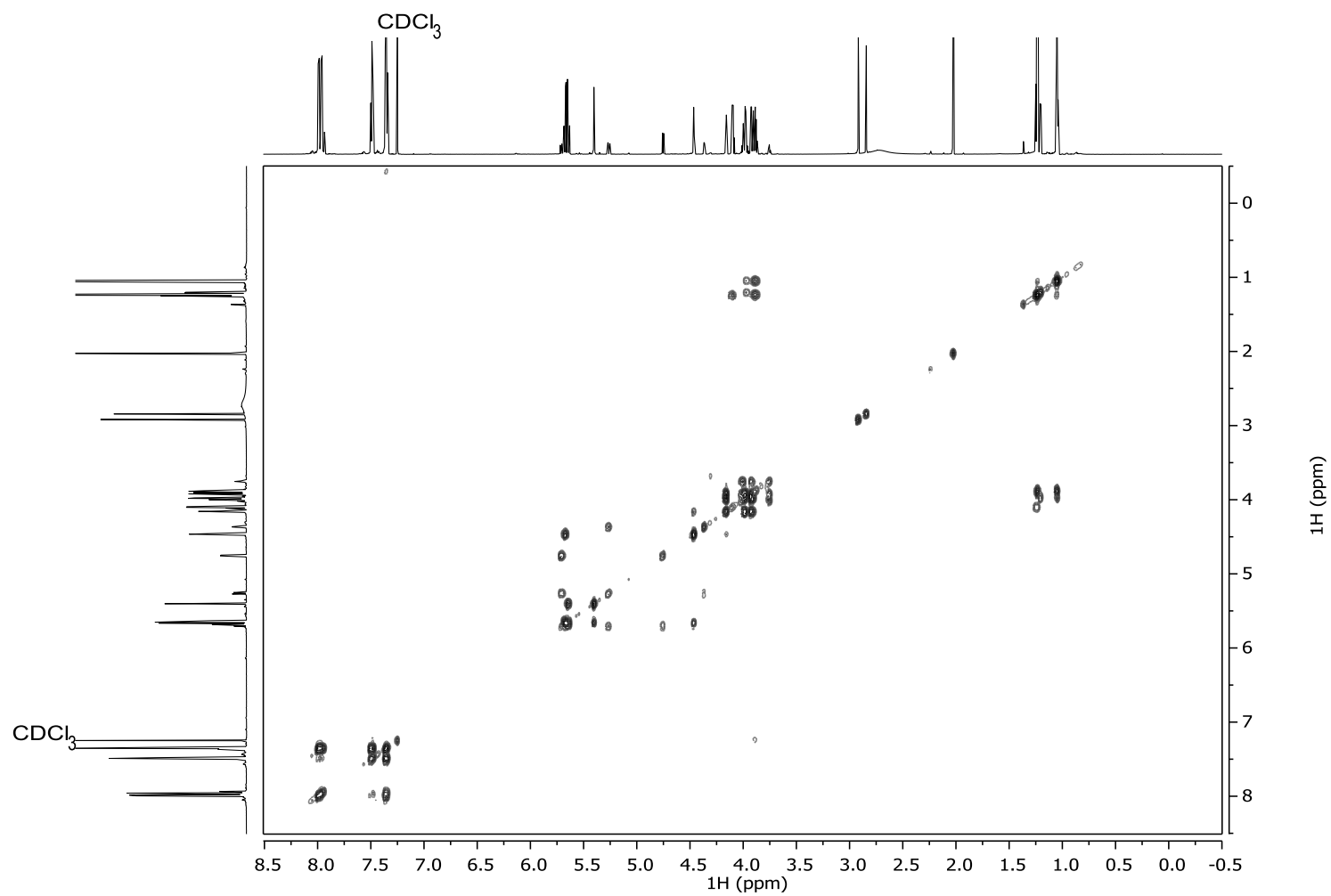
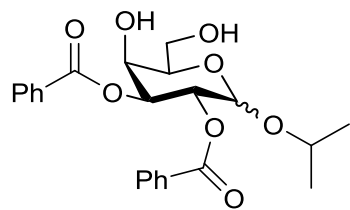
α+β peak normalized to 1 proton



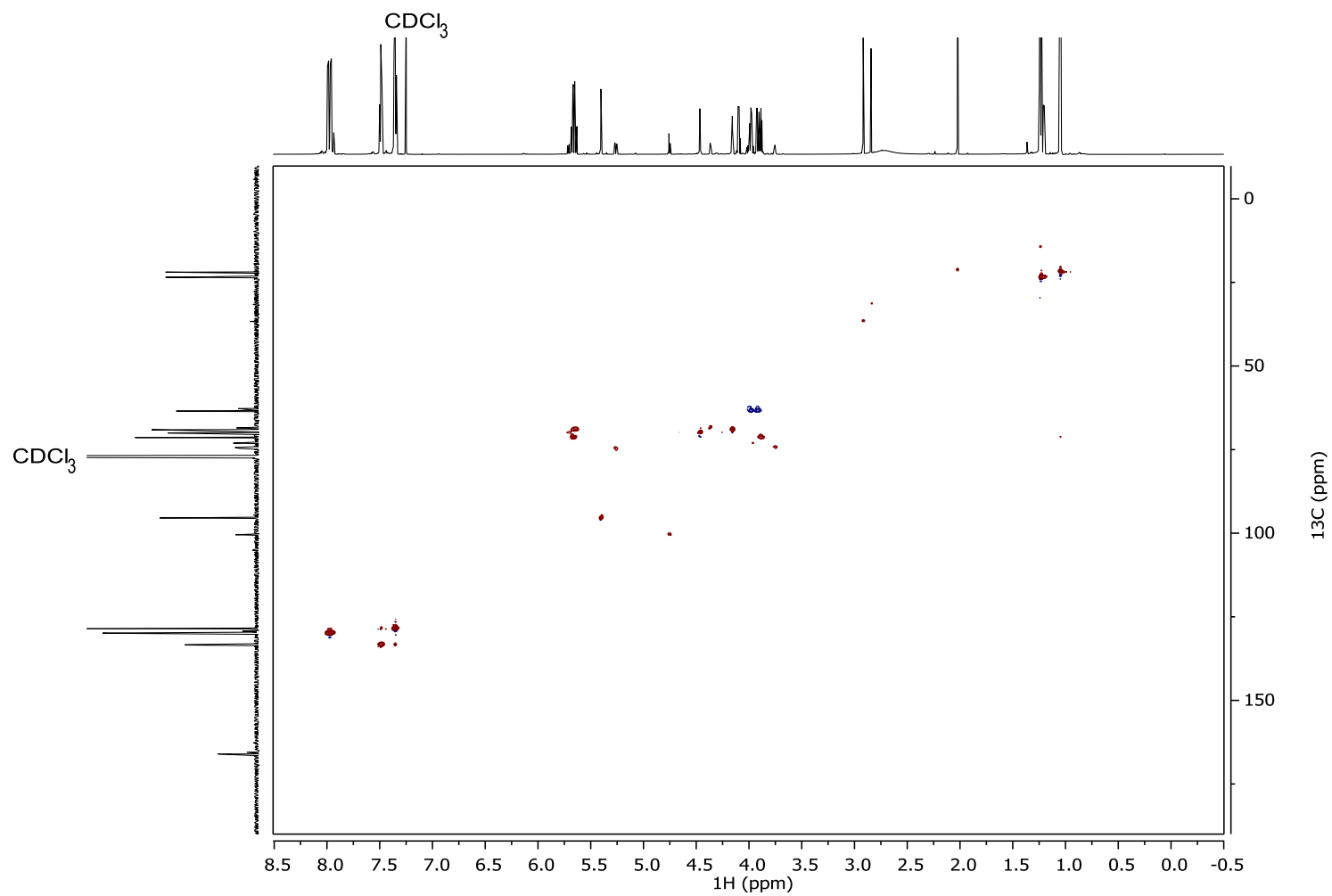
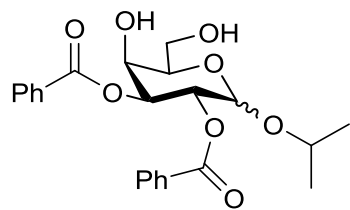
^{13}C NMR (126 MHz, CDCl_3) Isopropyl 2,3-di-*O*-benzoyl-D-galactopyranoside (6a)



^1H - ^1H COSY NMR (700 MHz, CDCl_3) Isopropyl 2,3-di-*O*-benzoyl-D-galactopyranoside (6a)

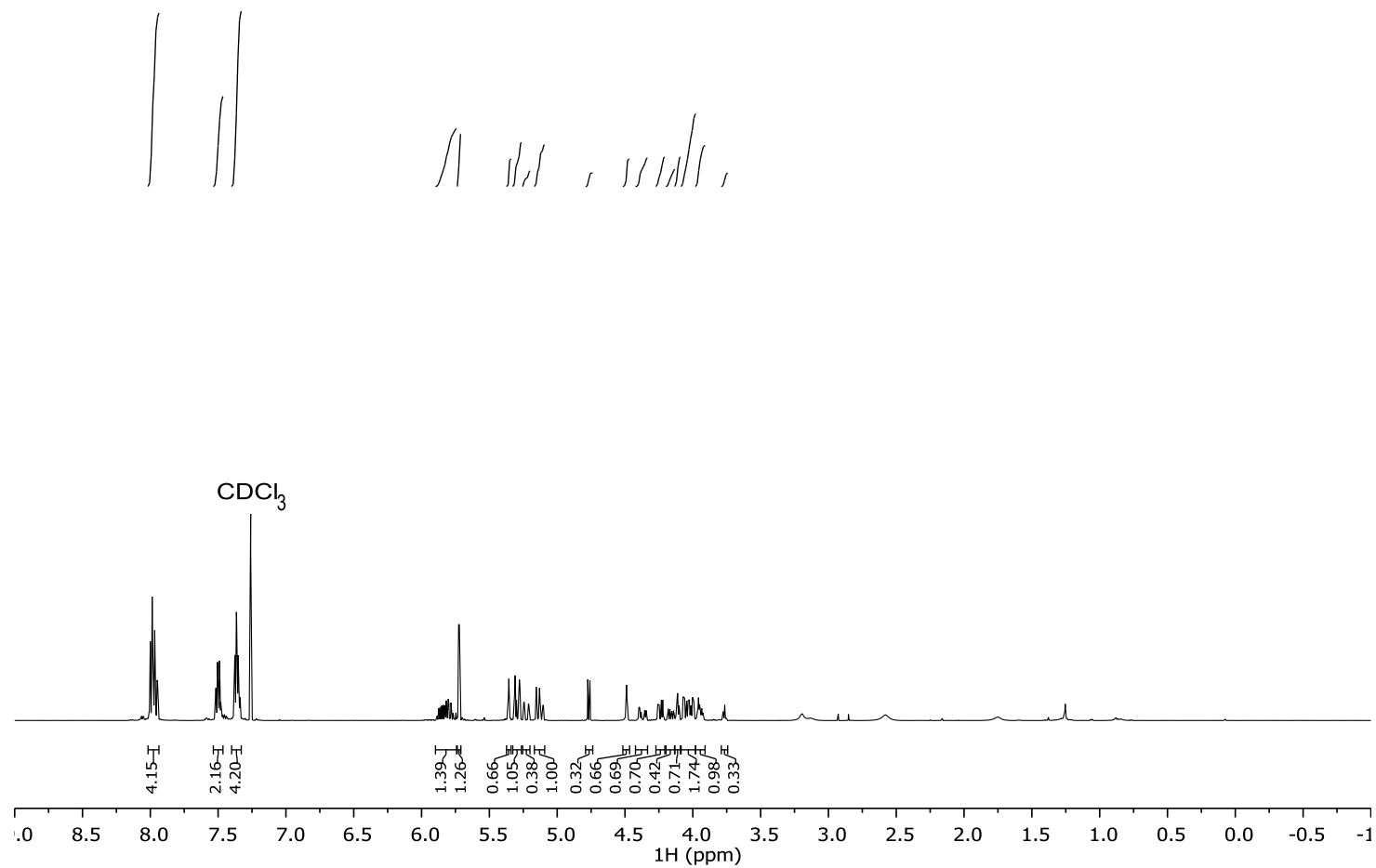
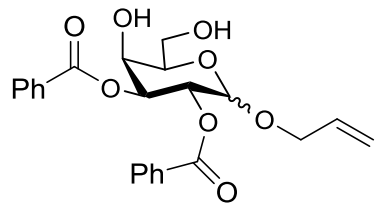


^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) Isopropyl 2,3-di-O-benzoyl-D-galactopyranoside (6a)



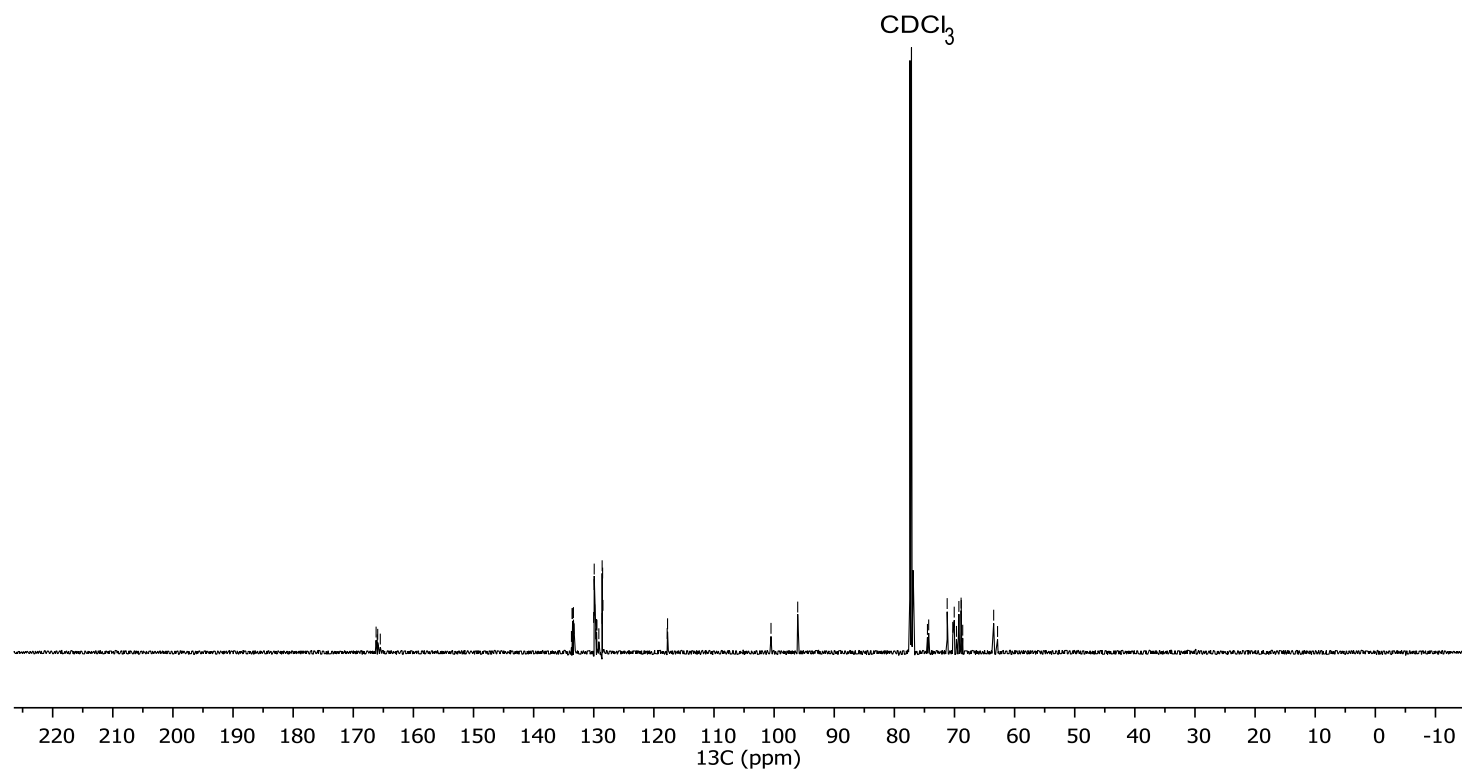
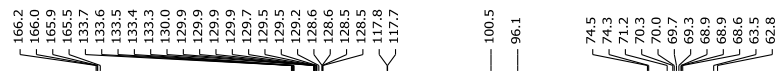
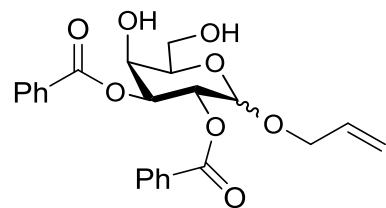
^1H NMR (500 MHz, CDCl_3) Allyl 2,3-di-O-benzoyl-D-galactopyranoside (6b)

$\alpha+\beta$ peak normalized to 1 proton

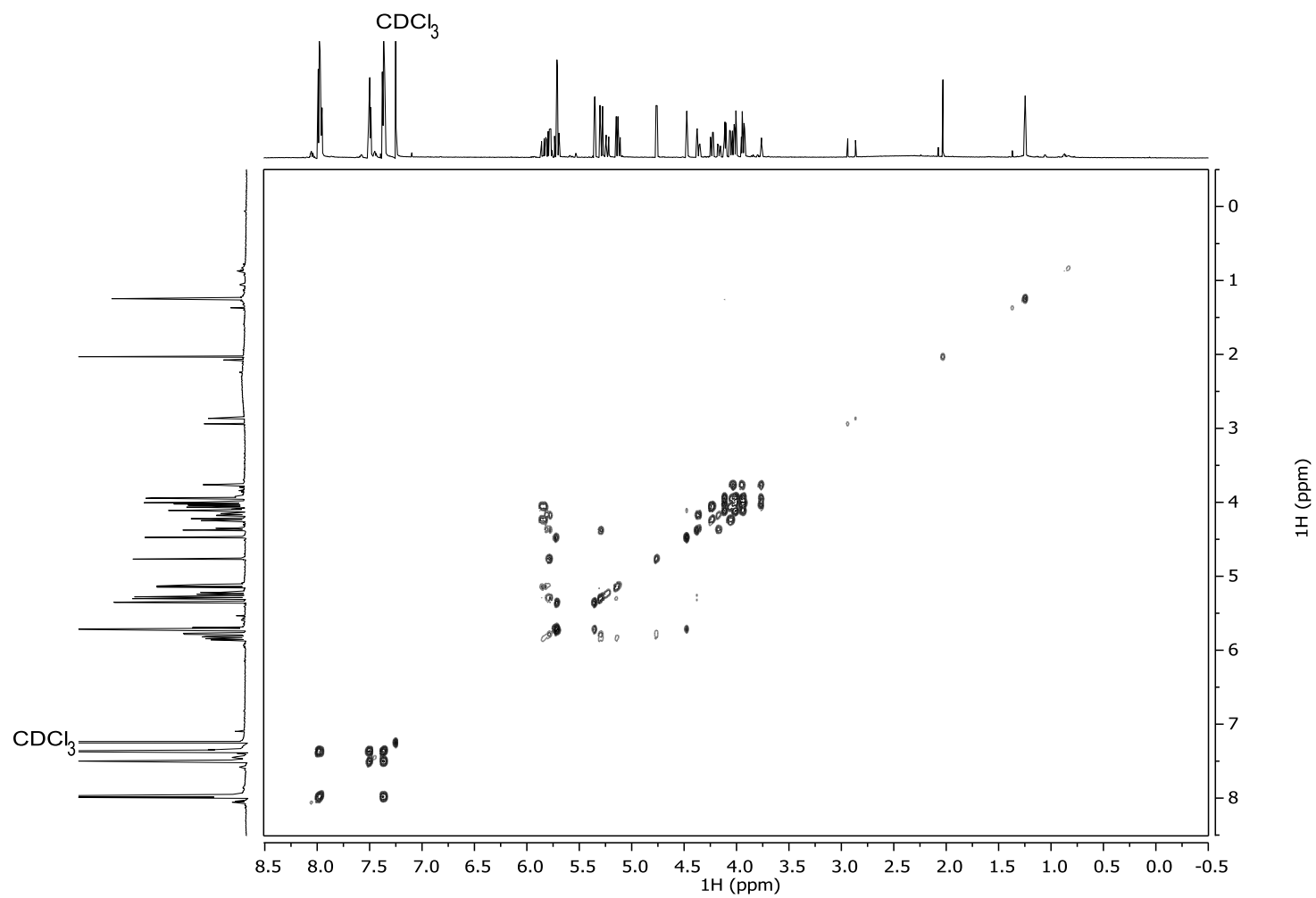
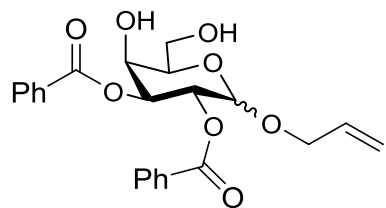


S157

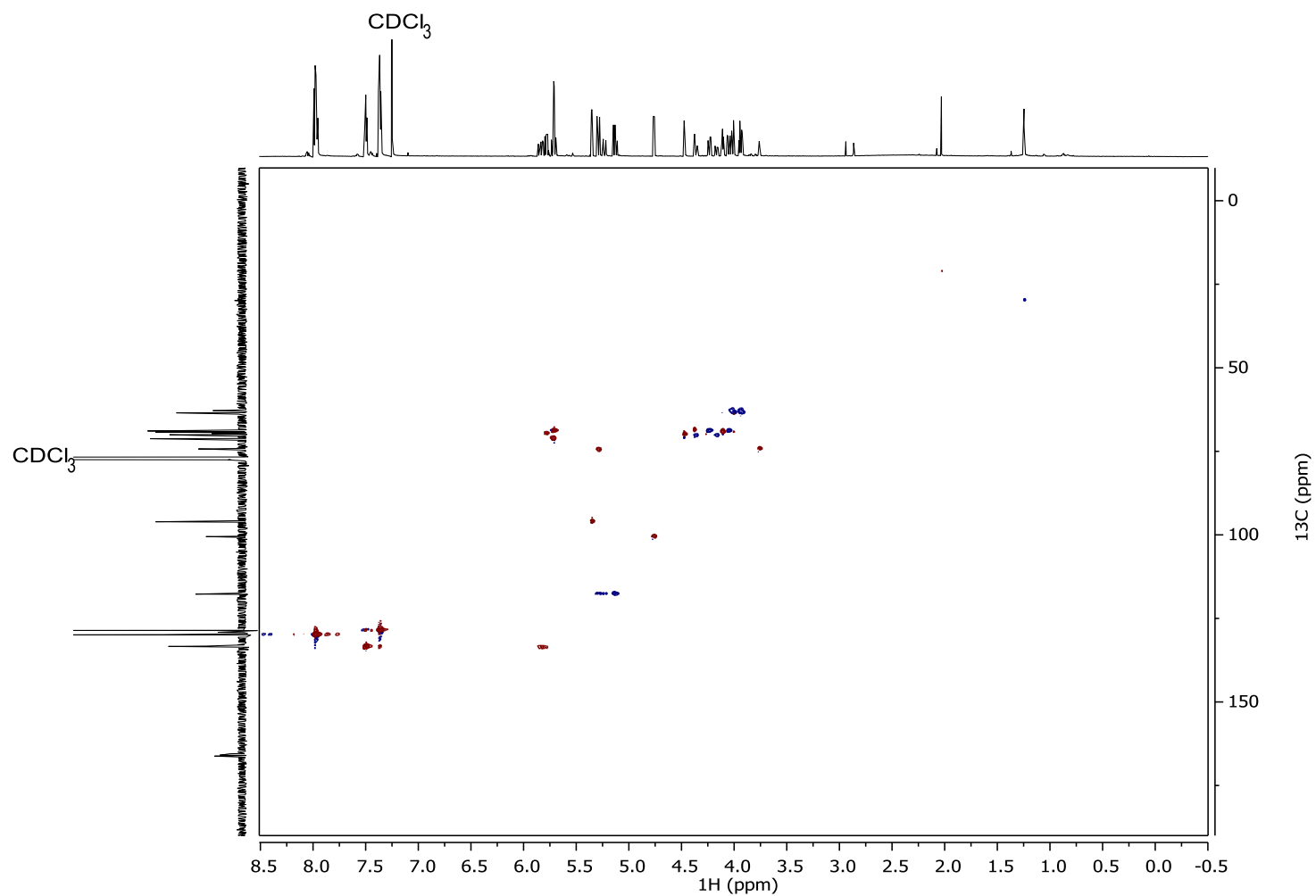
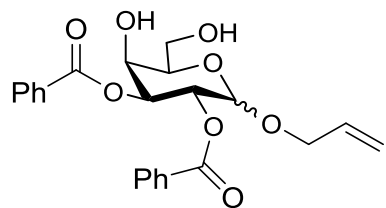
^{13}C NMR (125 MHz, CDCl_3) Allyl 2,3-di-O-benzoyl-D-galactopyranoside (6b)



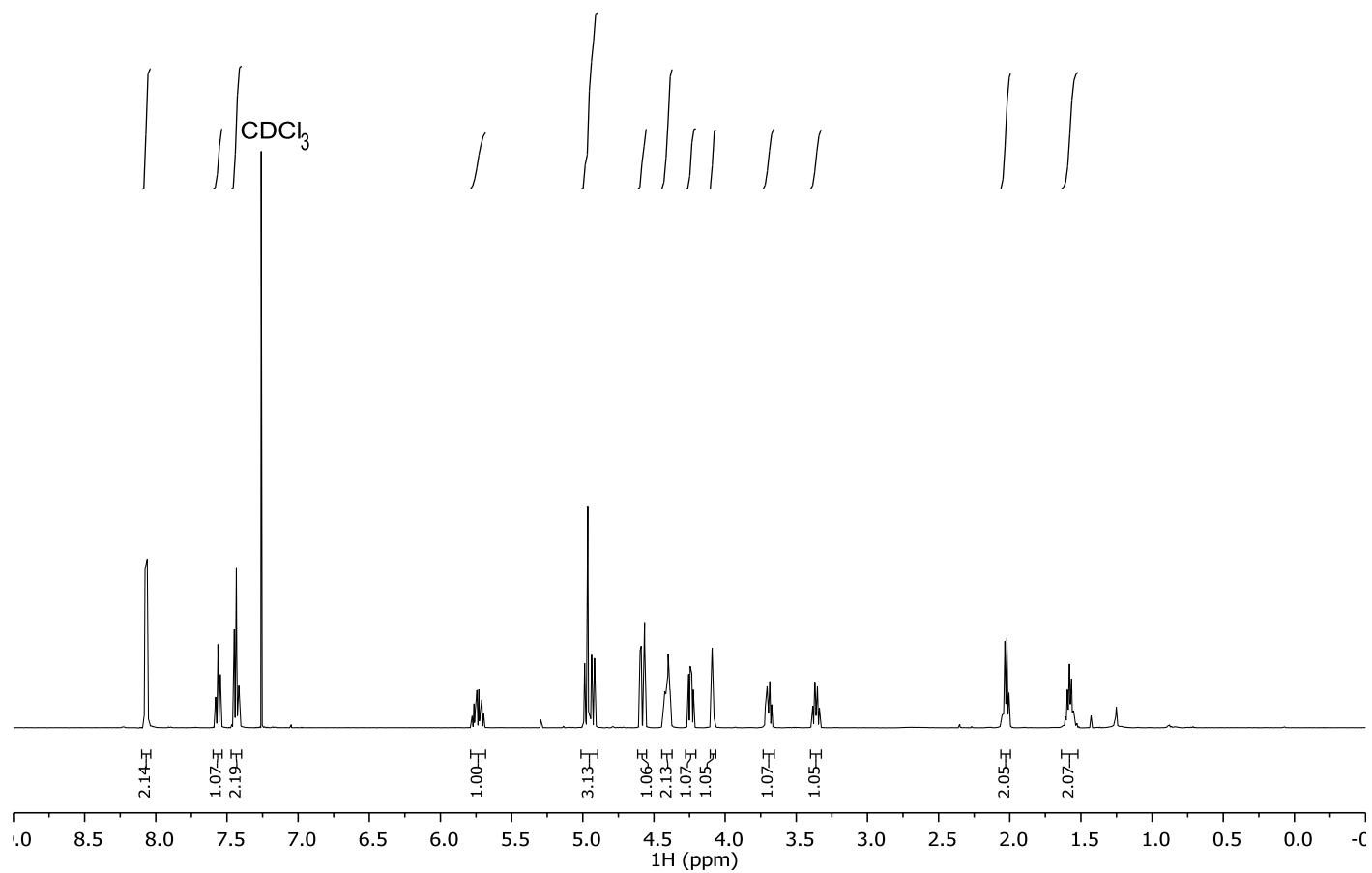
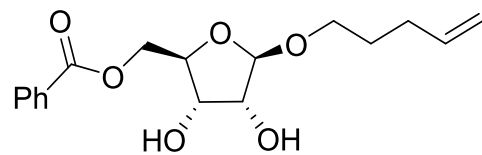
^1H - ^1H COSY NMR (700 MHz, CDCl_3) Allyl 2,3-di-O-benzoyl-D-galactopyranoside (6b)



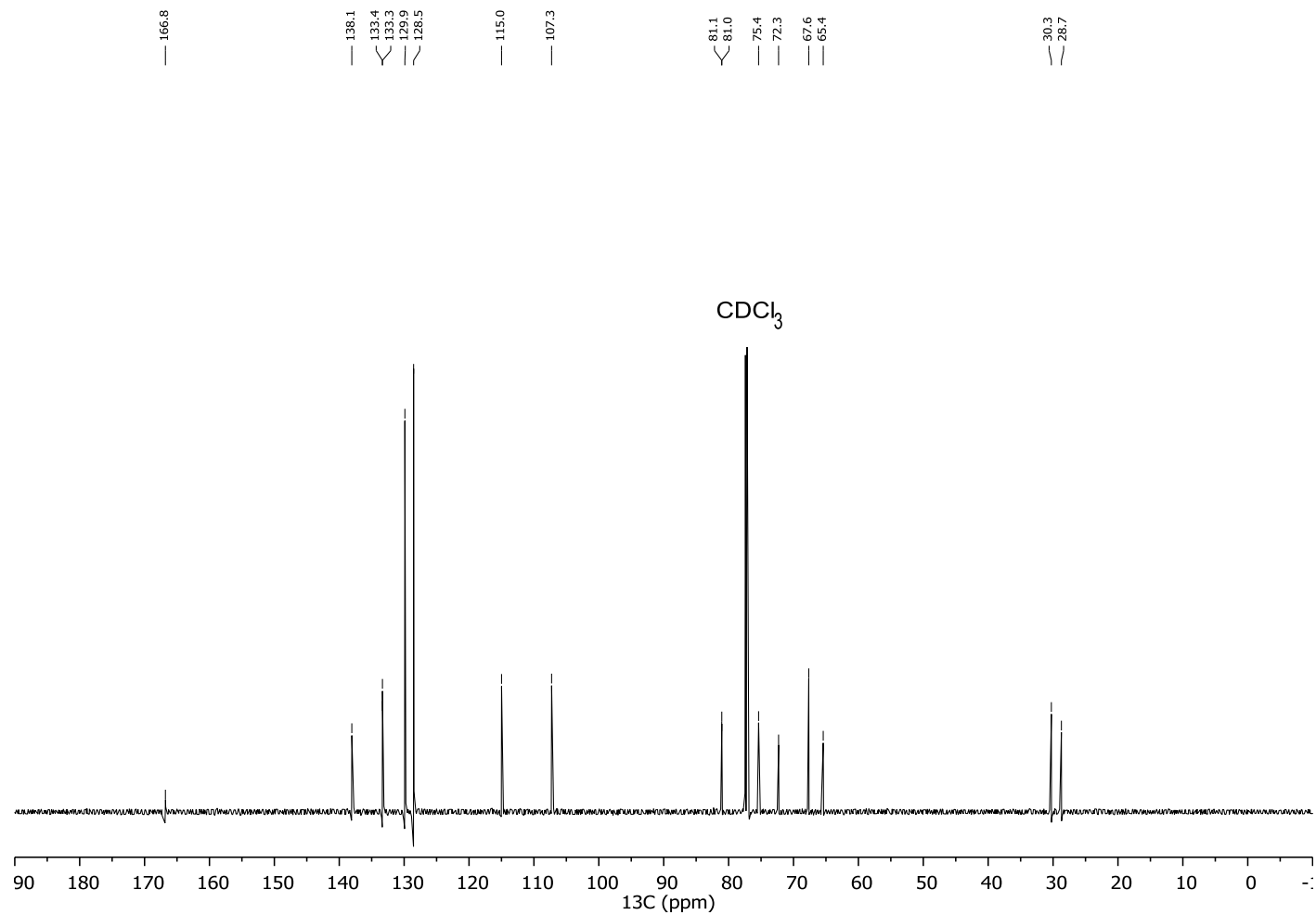
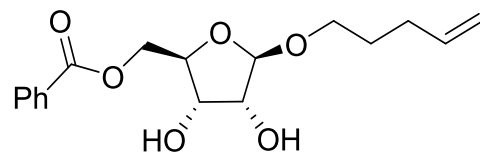
^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) Allyl 2,3-di-*O*-benzoyl-D-galactopyranoside (6b)



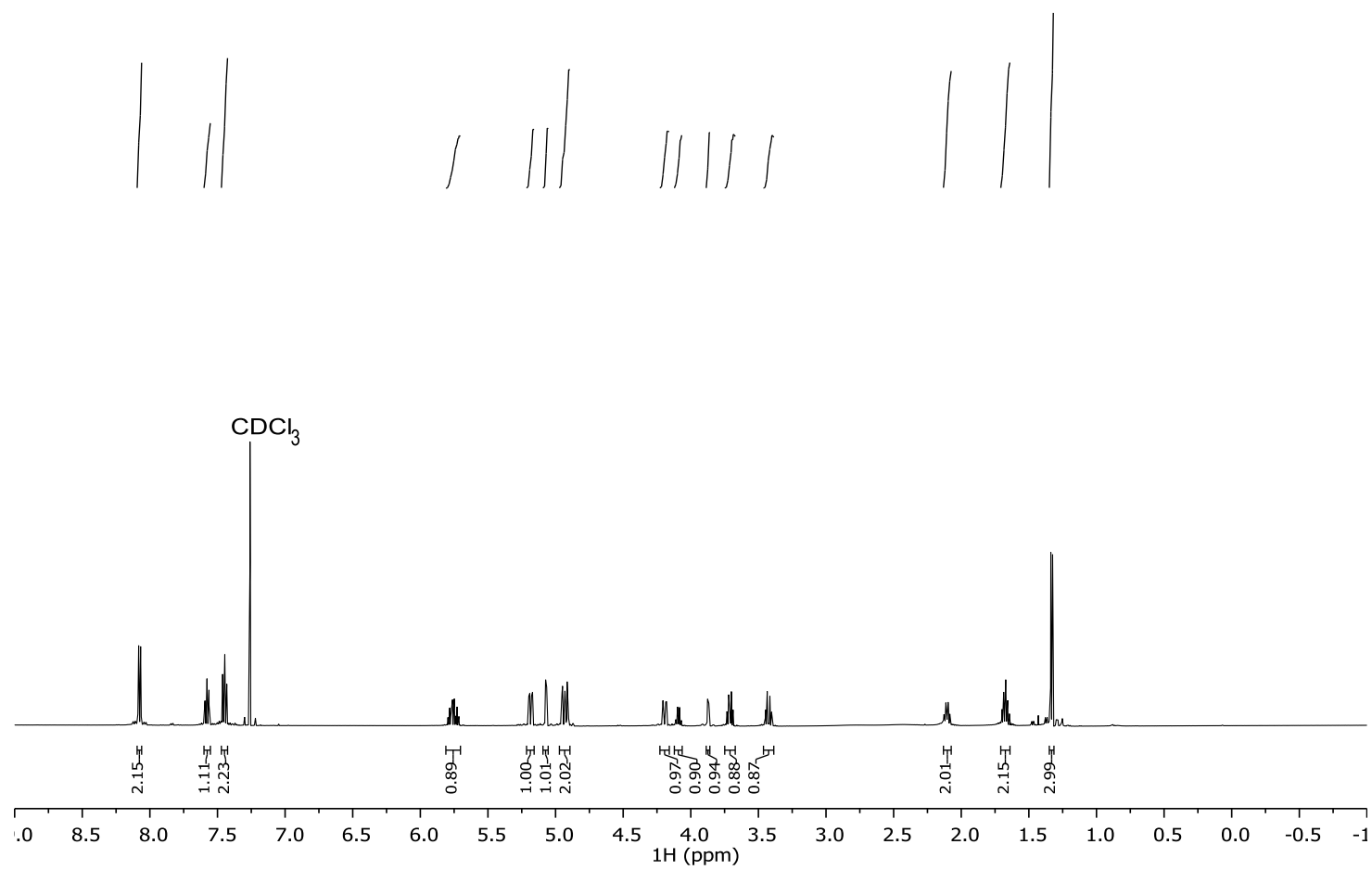
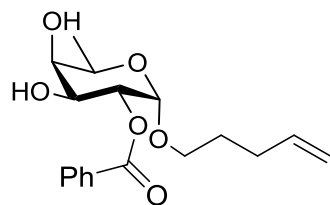
^1H NMR (500 MHz, CDCl_3) *n*-pentenyl 5-*O*-benzoyl- β -D-ribofuranoside (5)



^{13}C NMR (126 MHz, CDCl_3) *n*-pentenyl 5-*O*-benzoyl- β -D-ribofuranoside (5)

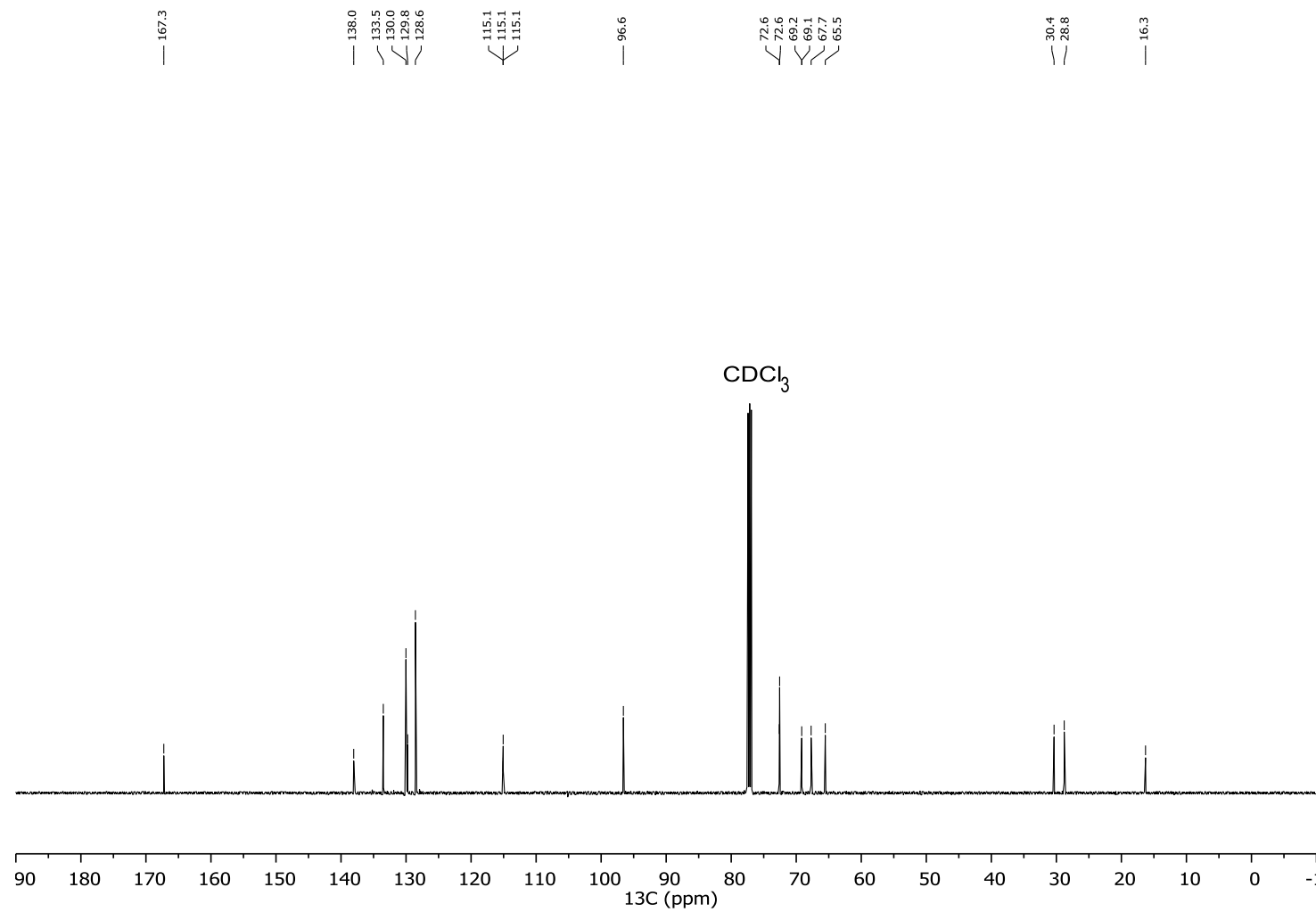
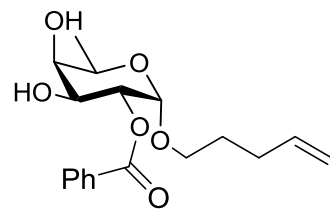


^1H NMR (500 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- α -D-fucopyranoside (α -6c)

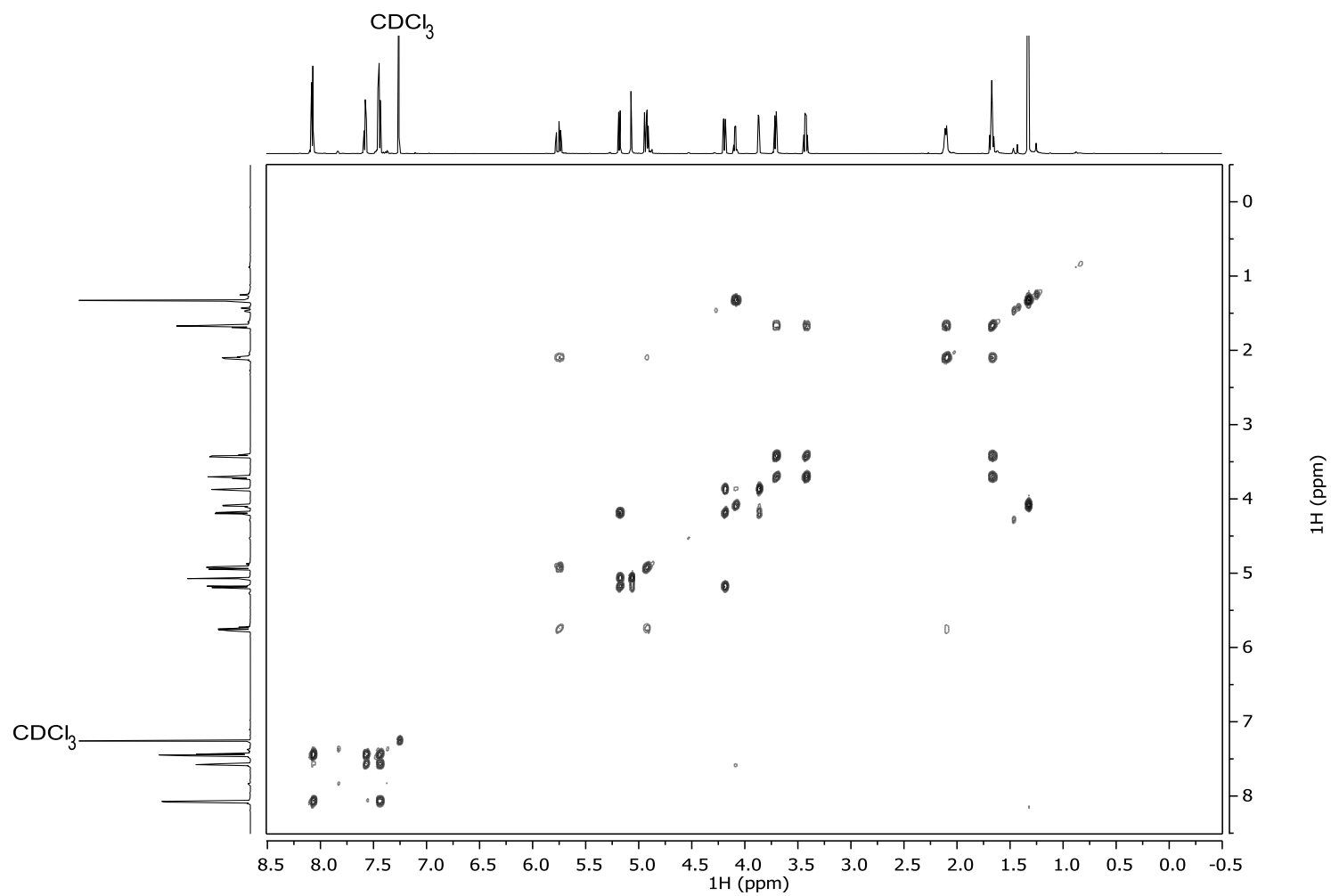
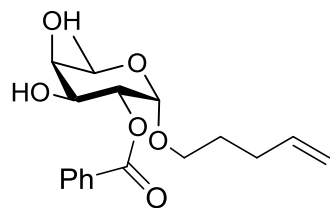


S163

^{13}C NMR (126 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- α -D-fucopyranoside (α -6c)

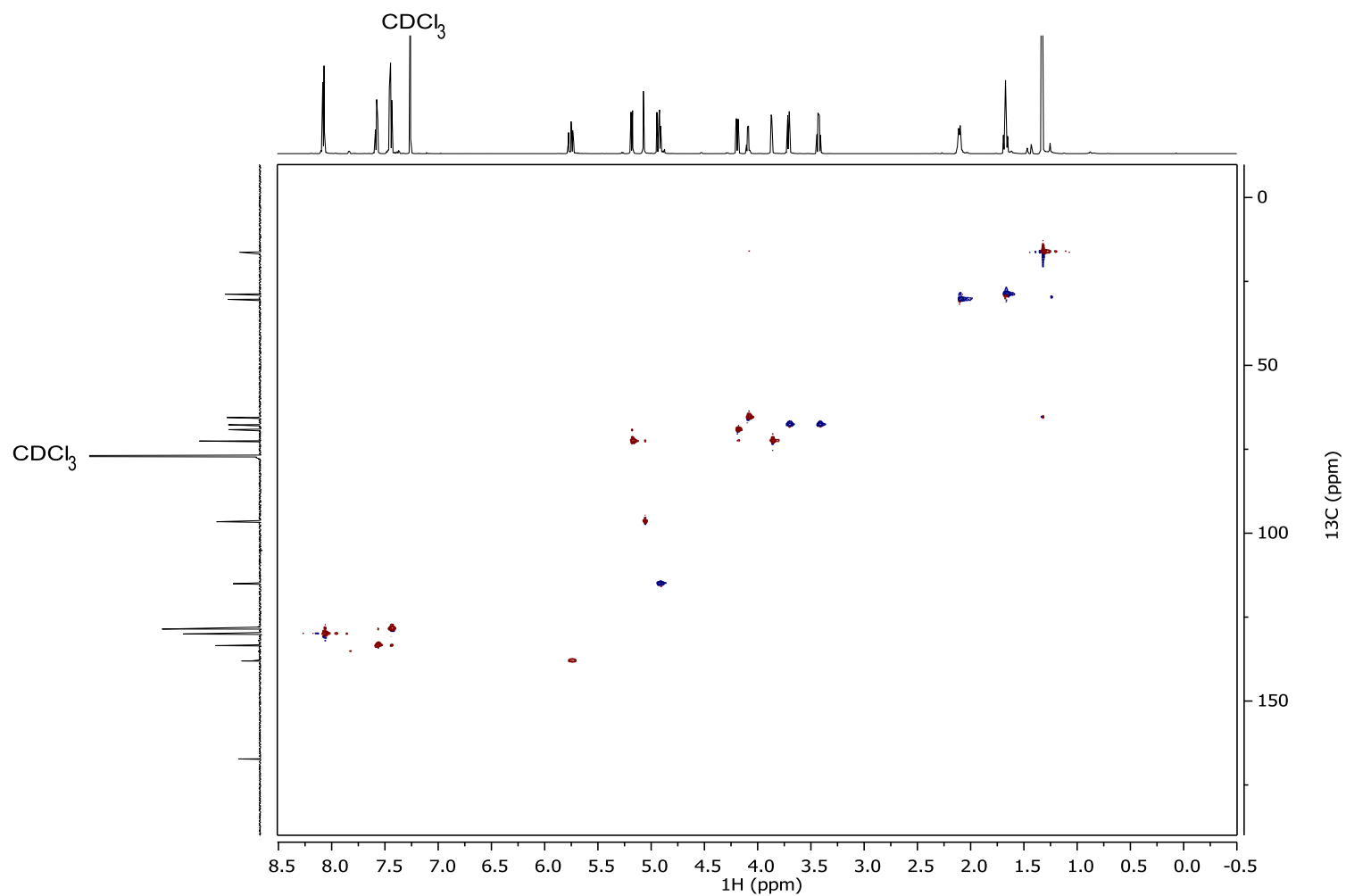
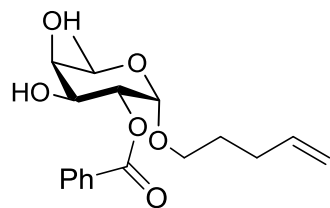


^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- α -D-fucopyranoside (α -6c)



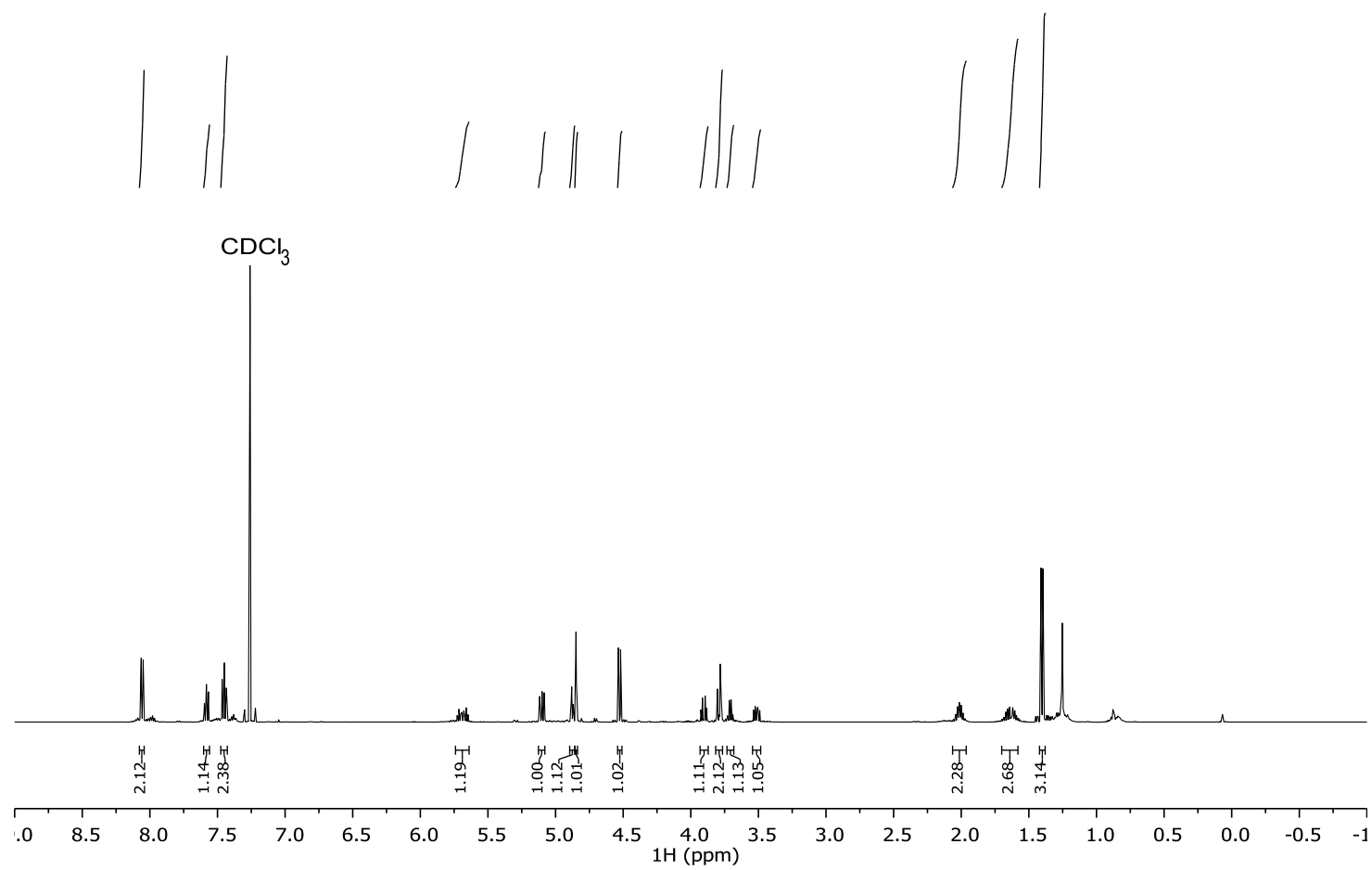
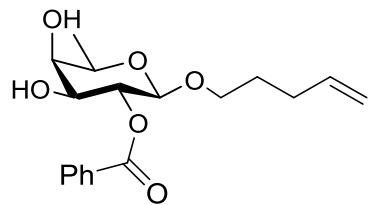
S165

^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- α -D-fucopyranoside (α -6c)

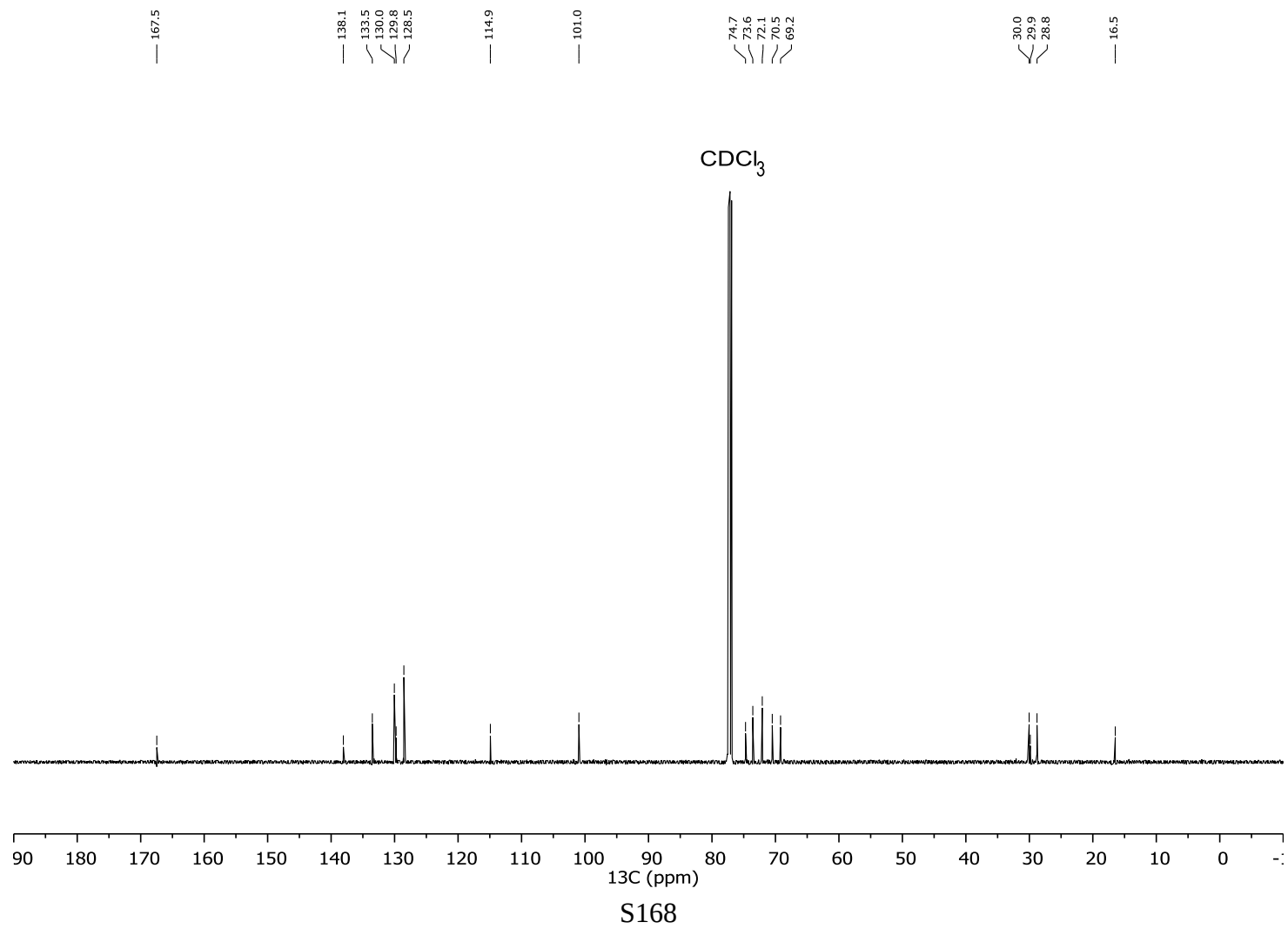
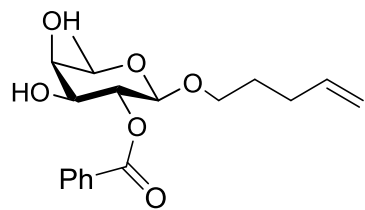


S166

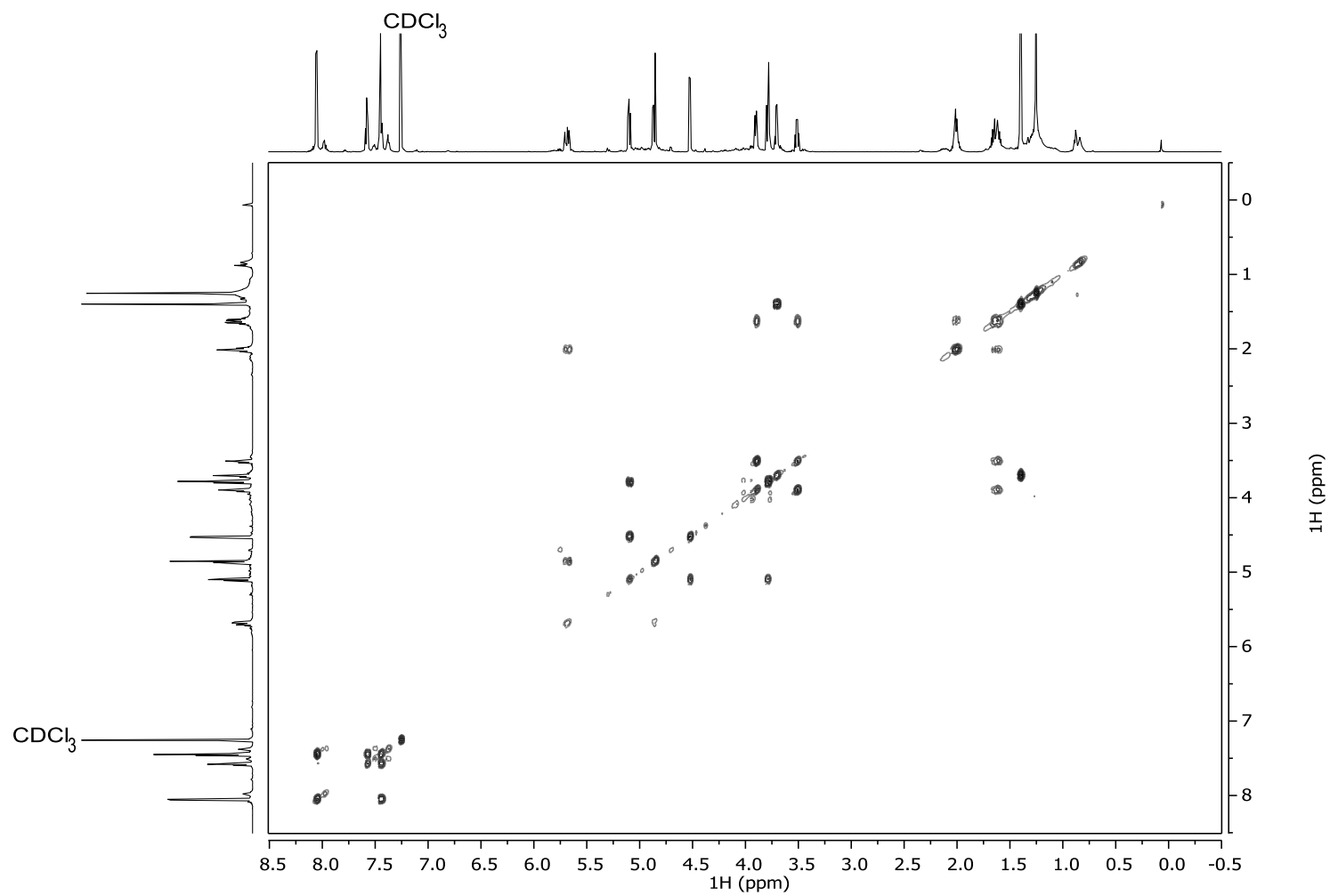
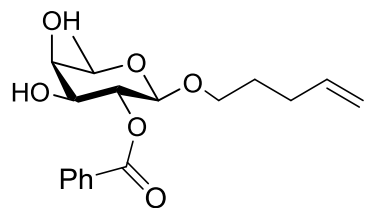
^1H NMR (500 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- β -D-fucopyranoside (β -6c)



^{13}C NMR (126 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- β -D-fucopyranoside (β -6c)



^1H - ^1H COSY NMR (700 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- β -D-fucopyranoside (β -6c)



S169

^1H - ^{13}C HSQC NMR (700 MHz, CDCl_3) *n*-pentenyl 2-O-benzoyl- β -D-fucopyranoside (β -6c)

