Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Short synthesis, X-ray and conformational analysis of a cyclic peracetylated L-sorbose-derived nitrone, a useful intermediate towards N-O-containing D-*gluco*-iminosugars

Salia Tangara,[a] Alice Kanazawa,*[a] Martine Fayolle,[a] Christian Philouze,[a] Jean-François Poisson,[a] Jean-Bernard Behr[b] and Sandrine Py*[a]

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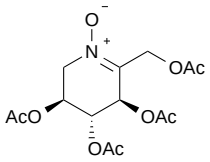
1- X-ray diffraction data for nitrone 4



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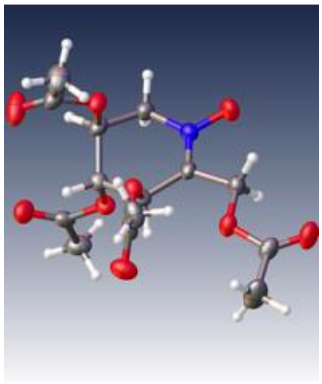
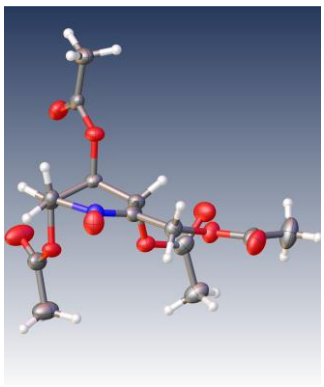




Single crystals of the compound were used for data collection on a Bruker-Enraf-Nonius kappaCCD diffractometer using Cu Ka graphite monochromated radiation (λ = 1.54178 Å) from a fine-focus sealed tube. Intensity data was corrected for absorption using SADABS and for Lorentz and polarization effects using EVAL. Subsequent merging was done using XPREP. Structure was solved by charge flipping method implement by SUPERFLIP. Refinements were performed with SHELX implemented via OLEX2. All non-hydrogen atoms were refined with anisotropic thermal parameters. The hydrogen atoms were generated in idealized positions, riding on the carrier atoms with isotropic thermal parameters and re-idealized before every refinement cycle. The crystal structure has been deposited at the Cambridge Cristallographic Data Center (CCDC 1587933). A summary of the crystallographic data and structure refinement is given in the following Table.

Crystal colour	colourless
Crystal habit	block
Crystal size, mm	0.50x0.44x0.40
Empirical formula	$C_{14}H_{19}NO_9$
a, Å	8.8584(18)
b, Å	7.6373(15)
c, Å	12.517(3)
!, deg	90
∀, deg	103.91(3)
#, deg	90
V, Å^3	822.0(3)
∀, Å	1.54178
Crystal system	monoclinic
Space group	$P2_1$
Z	2
T, k	200
Type of diffractometer	Bruker-Enraf-Nonius kappaCCD
method of data collection	phi and omega scans
Reflections collected	19394
Independent reflections [I > 2 #(I)]	2838 [R(int) = 0.0208]
Diffraction range, deg	3.638 to 67.975
Absorption correction	multi-scan
R [I >2 #(I)] w = 1/[s^2(Fo)^2+(0.0977P)^2+1.2107P] where P = ((Fo)^2+2(FC)^2)/3	R_1 = 0.0564 wR_2 = 0.1798
Number of parameters	222
Refinement method	Full-matrix least-squares on F^2

2- DFT calculations on nitrones 4 and 1 conformers

Computational method: Calculations were carried out using the density functional theory as implemented in the program package Gaussian09[1] with the 6-31+G(d,p) basis set and the Truhlar's functional M06-2X exchange–correlation functional.[2] Nitrones were previously studied at this level of theory and calculations well reproduced experimental data.[3] Each conformer was submitted to vibrational analysis and minima were characterized by the absence of imaginary frequencies. Thermodynamic analysis was carried out for a temperature of 298.15 K and a pressure of 1 atm, using the principal isotope for each element type. Cartesian (x,y,z) coordinates of optimized structures are provided below with corresponding zero-point energies and free enthalpies in hartrees.

Cartesian coordinates of the optimized structure of « all-axial acetates » conformer of 4 (from crystal structure)
E_0 = !1275.890897 Ha; G_{298} = !1275.948688 Ha

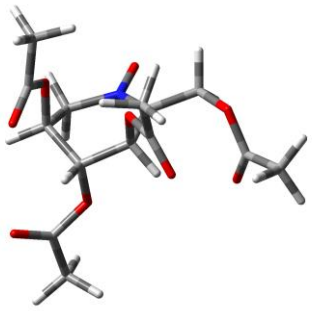


Figure S1. « All-axial acetates » conformer of nitrone **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.489836	1.356099	-0.309788
2	8	0	1.110797	-1.840842	-0.687030
3	8	0	1.914459	1.284033	1.075962
4	8	0	-0.114433	-1.062201	3.367410
5	8	0	-2.984824	0.075209	0.746196
6	7	0	0.210768	-0.762846	2.169709
7	8	0	-1.699548	1.000488	-2.181051
8	8	0	-2.966225	-2.034574	-0.025176
9	8	0	3.077394	-1.701165	-1.768827
10	6	0	2.146731	-2.365282	-1.390221
11	6	0	-3.405558	-0.911864	-0.082492

[1] Gaussian 09, Revision 4.2.0, M. J. Frisch, G. W. Trucks, H .B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A .F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
[2] Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.* 2008, **41**, 157–167.
[3] (a) Y. Lan, L. Zou, Y. Cao and K. N. Houk, *J. Phys. Chem. A*, 2011, **115**, 13906–13920; (b) Y. Salehi and M. Hamzehloueian, *Tetrahedron*, 2017, **73**, 4634–4643.

12	8	0	2.602045	2.059261	-0.922736
13	6	0	1.116333	-0.423730	-0.495805
14	1	0	1.419371	0.078384	-1.416040
15	6	0	2.061440	-0.079072	0.662250
16	1	0	3.098577	-0.273803	0.373039
17	6	0	-0.669988	-0.400538	1.285063
18	6	0	-0.317263	-0.062968	-0.129340
19	1	0	-0.987441	-0.591213	-0.812273
20	6	0	2.188038	2.265742	0.190856
21	6	0	-1.183211	1.760736	-1.399100
22	6	0	1.659906	-0.888123	1.877575
23	1	0	1.864740	-1.952526	1.748192
24	1	0	2.158200	-0.528143	2.777736
25	6	0	-2.082958	-0.319295	1.781284
26	1	0	-2.376244	-1.284036	2.207125
27	1	0	-2.160701	0.439597	2.564660
28	6	0	1.952970	-3.838133	-1.608325
29	1	0	1.808223	-4.339601	-0.648630
30	1	0	2.822612	-4.242128	-2.122891
31	1	0	1.050650	-4.000303	-2.202899
32	6	0	-1.196560	3.259550	-1.491699
33	1	0	-1.579241	3.686187	-0.561620
34	1	0	-1.814688	3.564100	-2.334096
35	1	0	-0.171281	3.613864	-1.634498
36	6	0	1.889829	3.610634	0.789345
37	1	0	0.820077	3.664133	1.010071
38	1	0	2.173885	4.391630	0.085934
39	1	0	2.429641	3.730505	1.731178
40	6	0	-4.431686	-0.414363	-1.057795
41	1	0	-5.154884	0.230912	-0.556602
42	1	0	-4.925750	-1.267927	-1.519051
43	1	0	-3.917887	0.170080	-1.826570

Cartesian coordinates of optimized structure of « all-equatorial acetates » conformer of 4
E_0 = !1275.890794 Ha; G_{298} = ! 275.947094 Ha

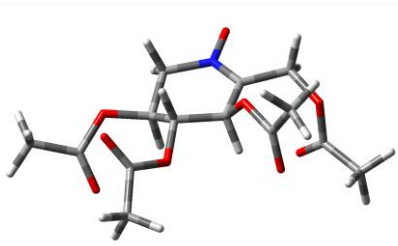


Figure *S2*. « All-equatorial acetates » conformer of nitrone **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.259960	-1.342277	-0.519700
2	6	0	-0.919063	-2.429066	-0.598581
3	6	0	-1.486764	-1.218128	0.127722
4	6	0	-0.861501	0.049656	-0.441949
5	6	0	0.653000	0.006329	-0.275980
6	1	0	-1.309423	-2.481340	-1.619039
7	1	0	-1.320766	-1.266805	1.209804
8	1	0	-1.128829	0.142919	-1.501165
9	1	0	0.909879	0.362151	0.728114
10	1	0	-1.166102	-3.358067	-0.084567
11	7	0	0.552846	-2.417819	-0.693931
12	8	0	1.074142	-3.552443	-0.962936
13	6	0	2.746915	-1.526913	-0.588587
14	1	0	2.998866	-2.458144	-0.072151
15	1	0	3.080022	-1.603972	-1.627272
16	8	0	3.464249	-0.425308	-0.030784
17	8	0	1.217889	0.909637	-1.239022
18	8	0	-2.883674	-1.277593	-0.153989
19	8	0	-1.271797	1.216083	0.263273
20	6	0	3.441637	-0.339325	1.323925
21	6	0	-3.745674	-0.691998	0.712397
22	6	0	4.374040	0.721205	1.829806
23	1	0	5.355403	0.610979	1.364319
24	1	0	3.968674	1.699892	1.560594
25	1	0	4.449619	0.637005	2.912568
26	8	0	2.737267	-1.049697	1.999312
27	6	0	1.893554	1.988501	-0.778117
28	6	0	2.489001	2.764138	-1.917325
29	1	0	3.320734	2.185447	-2.329702
30	1	0	1.751846	2.906142	-2.709368
31	1	0	2.854514	3.721426	-1.550220
32	8	0	2.008762	2.257084	0.391752
33	6	0	-2.382364	1.869989	-0.143360
34	8	0	-3.028633	1.543559	-1.110396
35	6	0	-2.696655	3.001517	0.788973
36	1	0	-1.790103	3.554754	1.039626
37	1	0	-3.441371	3.652032	0.333745
38	1	0	-3.094414	2.566531	1.711222
39	6	0	-5.143300	-0.726544	0.170560
40	1	0	-5.367292	-1.703738	-0.259920
41	1	0	-5.846040	-0.478034	0.963966
42	1	0	-5.200848	0.020747	-0.627420
43	8	0	-3.397081	-0.189785	1.752248

Cartesian coordinates of the optimized structure of « all-axial benzyloxy groups » conformer of nitrone 1

E_0 = !1746.169132 Ha; G_{298} = !1746.24112 Ha

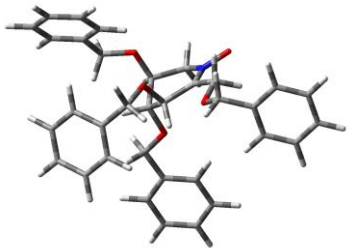


Figure S3. « All-axial benzyloxy groups » conformer of nitrone **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.475382	-1.503526	-0.318495
2	8	0	-0.235921	2.003506	0.534570
3	8	0	-1.876229	-0.792586	2.205448
4	8	0	2.027271	-0.792356	3.189549
5	8	0	2.433940	-1.548515	-0.750943
6	7	0	1.137595	-0.417949	2.349518
7	6	0	-0.834060	0.723429	0.621706
8	1	0	-1.726046	0.672960	-0.014802
9	6	0	-1.202620	0.441279	2.083155
10	1	0	-1.832592	1.260280	2.467001
11	6	0	1.219914	-0.686635	1.082250
12	6	0	0.167804	-0.303335	0.084434
13	1	0	0.671826	0.157224	-0.776338
14	6	0	0.047939	0.391393	2.935952
15	1	0	0.460542	1.391880	3.086316
16	1	0	-0.157826	-0.067670	3.903113
17	6	0	2.409983	-1.489192	0.661570
18	1	0	3.322820	-1.031039	1.068842
19	1	0	2.341790	-2.499980	1.098299
20	6	0	-3.238089	-0.748753	1.833088
21	1	0	-3.850596	-0.507595	2.715426
22	1	0	-3.411760	0.043048	1.087711
23	6	0	-3.677392	-2.059463	1.229428
24	6	0	-5.011699	-2.205364	0.838670
25	6	0	-2.775633	-3.096325	0.995424
26	6	0	-5.438645	-3.365313	0.198502
27	1	0	-5.718461	-1.397836	1.021926
28	6	0	-3.206403	-4.261659	0.358693
29	1	0	-1.737810	-2.964809	1.278582
30	6	0	-4.532057	-4.398222	-0.047905
31	1	0	-6.475213	-3.464328	-0.109212
32	1	0	-2.497100	-5.063352	0.175211
33	1	0	-4.860235	-5.303250	-0.549658
34	6	0	3.402165	-2.451485	-1.244348
35	1	0	3.225533	-3.456344	-0.830702
36	1	0	3.232576	-2.494963	-2.325250
37	6	0	4.823484	-2.021135	-0.952562
38	6	0	5.756532	-2.925052	-0.446461
39	6	0	5.215157	-0.701190	-1.196591
40	6	0	7.070217	-2.524551	-0.199606

41	1	0	5.453812	-3.948181	-0.236166
42	6	0	6.522156	-0.296424	-0.943366
43	1	0	4.482296	0.007150	-1.574591
44	6	0	7.454579	-1.209487	-0.447034
45	1	0	7.787093	-3.236645	0.197176
46	1	0	6.815881	0.731733	-1.131774
47	1	0	8.473767	-0.893265	-0.247902
48	6	0	-1.152568	3.031682	0.221312
49	1	0	-1.973748	3.049347	0.956798
50	1	0	-1.600954	2.835547	-0.765259
51	6	0	-0.456332	4.369067	0.218378
52	6	0	0.895754	4.495299	0.534154
53	6	0	-1.193693	5.511666	-0.107120
54	6	0	1.501350	5.752838	0.524956
55	1	0	1.466940	3.608052	0.784419
56	6	0	-0.589623	6.764637	-0.115471
57	1	0	-2.249171	5.417816	-0.355110
58	6	0	0.763939	6.888630	0.201760
59	1	0	2.554671	5.841767	0.772907
60	1	0	-1.172836	7.644209	-0.370027
61	1	0	1.238062	7.865080	0.196125
62	6	0	-0.682368	-1.627269	-1.720392
63	1	0	-1.002102	-2.663327	-1.865875
64	1	0	0.271266	-1.470918	-2.243342
65	6	0	-1.743364	-0.674001	-2.218726
66	6	0	-3.090620	-0.948070	-1.956546
67	6	0	-1.403420	0.524232	-2.850051
68	6	0	-4.076926	-0.024079	-2.290530
69	1	0	-3.361212	-1.885286	-1.474448
70	6	0	-2.390589	1.449338	-3.194015
71	1	0	-0.359009	0.740882	-3.064776
72	6	0	-3.727529	1.180666	-2.905205
73	1	0	-5.118055	-0.247450	-2.075496
74	1	0	-2.114576	2.378740	-3.683614
75	1	0	-4.496236	1.901075	-3.168198

Cartesian coordinates of optimized structure of « all-equatorial benzyloxy groups » conformer of nitrone 1

E_0 = !1746.166909 Ha; G_{298} = !1746.240326 Ha

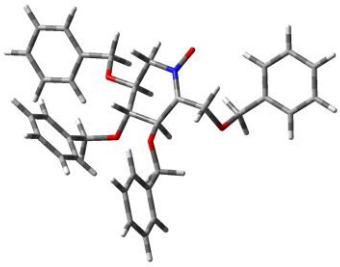


Figure *S4*. « All-equatorial benzyloxy groups » conformer of nitrone **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.519074	-0.719224	0.534246
2	6	0	0.381361	-2.141257	1.076785
3	6	0	1.110015	-1.550672	-0.127641
4	6	0	0.833699	-0.058447	-0.197672
5	6	0	-0.663481	0.171650	-0.331963
6	1	0	0.838086	-1.788364	2.007298
7	1	0	0.757804	-2.027907	-1.059183
8	1	0	1.179271	0.414174	0.734512
9	1	0	-0.936492	-0.021779	-1.381904
10	1	0	0.384222	-3.231694	1.079318
11	7	0	-1.055628	-1.780149	1.131256
12	8	0	-1.758997	-2.591243	1.827929
13	6	0	-2.987723	-0.396994	0.587641
14	1	0	-3.500385	-1.075237	1.275178
15	1	0	-3.114288	0.636061	0.920657
16	8	0	-3.530254	-0.457853	-0.724015
17	6	0	-3.706865	-1.795205	-1.184388
18	1	0	-3.862685	-1.708141	-2.263413
19	1	0	-2.788659	-2.378093	-1.011421
20	8	0	-0.955116	1.516915	-0.012858
21	8	0	2.501692	-1.728840	0.002410
22	8	0	1.421892	0.557583	-1.320214
23	6	0	-1.422365	2.286497	-1.105356
24	1	0	-0.684537	2.246103	-1.921570
25	1	0	-2.368454	1.863775	-1.477184
26	6	0	2.953845	-3.067405	-0.141217
27	1	0	2.456173	-3.524506	-1.011166
28	1	0	2.703598	-3.662922	0.747370
29	6	0	2.755405	1.040312	-1.153867
30	1	0	2.992968	1.498721	-2.118863
31	1	0	3.444531	0.208177	-0.978759
32	6	0	4.445771	-3.041400	-0.340224
33	6	0	5.305045	-3.655407	0.569294
34	6	0	4.981753	-2.381520	-1.450433
35	6	0	6.686149	-3.617740	0.372858
36	1	0	4.893783	-4.161953	1.438776
37	6	0	6.358297	-2.336532	-1.645906
38	1	0	4.310160	-1.901814	-2.158616
39	6	0	7.213706	-2.957231	-0.733200
40	1	0	7.347450	-4.098383	1.087010
41	1	0	6.766840	-1.822869	-2.510670
42	1	0	8.287827	-2.924385	-0.886265
43	6	0	2.883835	2.056784	-0.043830
44	6	0	2.034163	3.166412	0.003084
45	6	0	3.848133	1.893035	0.951469
46	6	0	2.156867	4.104366	1.023992
47	1	0	1.265177	3.286940	-0.756480
48	6	0	3.980711	2.836930	1.970784
49	1	0	4.491720	1.016425	0.929817
50	6	0	3.135396	3.943440	2.007288
51	1	0	1.487170	4.959023	1.049983
52	1	0	4.736014	2.701832	2.738811
53	1	0	3.234114	4.677625	2.800975
54	6	0	-1.627441	3.714590	-0.667155
55	6	0	-1.360636	4.128380	0.637689

56	6	0	-2.094288	4.647710	-1.598510
57	6	0	-1.560931	5.460489	1.004732
58	1	0	-0.989704	3.405690	1.356588
59	6	0	-2.291853	5.975225	-1.232499
60	1	0	-2.305884	4.329992	-2.617455
61	6	0	-2.024946	6.386488	0.074498
62	1	0	-1.351982	5.771964	2.024189
63	1	0	-2.656241	6.689063	-1.964834
64	1	0	-2.180703	7.421368	0.362804
65	6	0	-4.885162	-2.479192	-0.533730
66	6	0	-6.182055	-2.158368	-0.947325
67	6	0	-4.704293	-3.402359	0.498782
68	6	0	-7.284716	-2.754423	-0.342755
69	1	0	-6.322349	-1.432560	-1.744785
70	6	0	-5.809527	-4.000092	1.106342
71	1	0	-3.697043	-3.630245	0.842645
72	6	0	-7.098202	-3.679560	0.685896
73	1	0	-8.287722	-2.501558	-0.672631
74	1	0	-5.660843	-4.714172	1.910365
75	1	0	-7.956821	-4.147477	1.157846

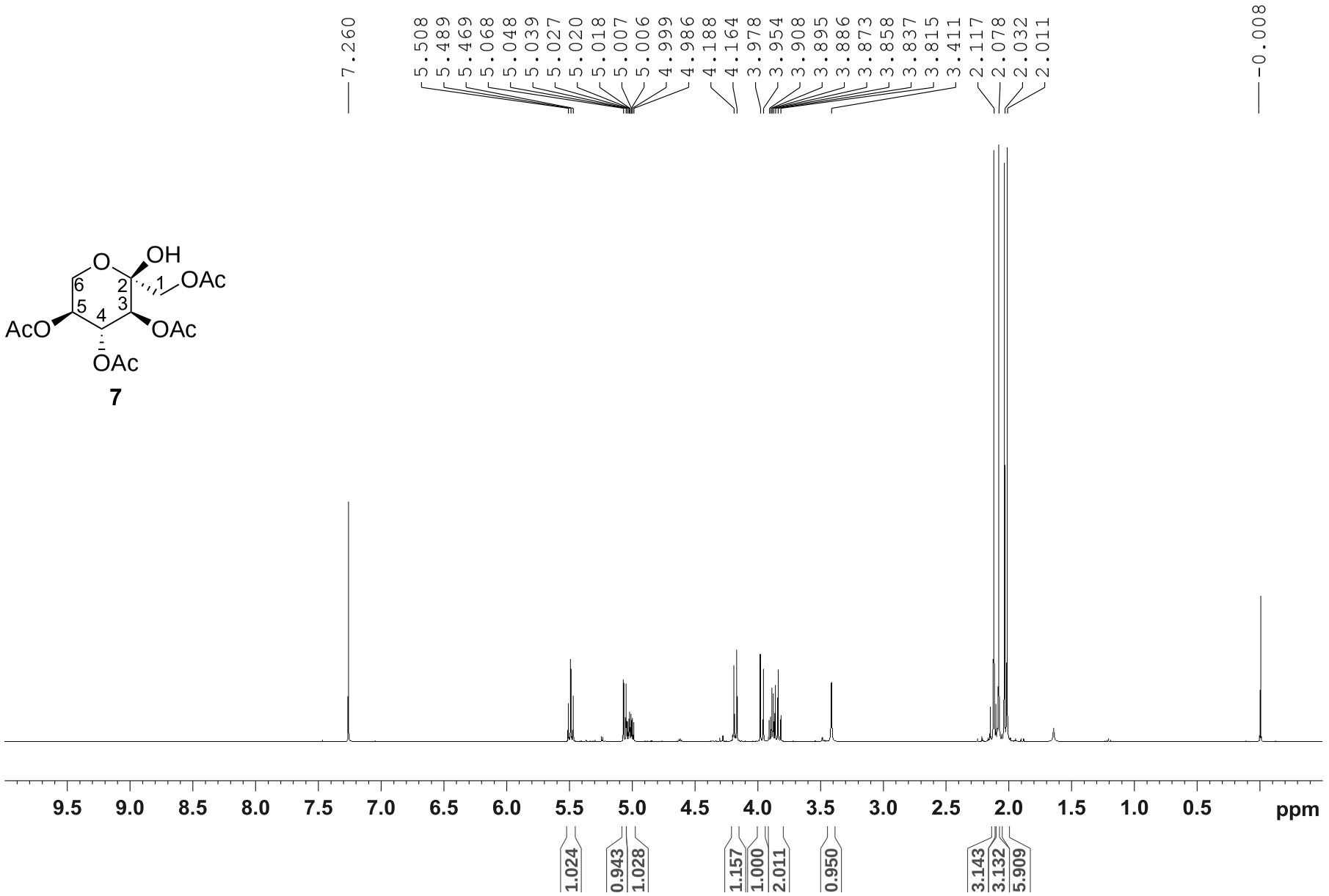
3- Glycosidase inhibition assays

α-Glucosidases (from rice and yeast), *β*-glucosidases (from almond and *Asp. niger*), *β*-galactosidase (from *Asp. oryzae*), ∃-mannosidase (from Jack bean), ∃-rhamnosidase (from *Asp. niger*) and *p*-nitrophenyl glycosides used for the bioassays were purchased from Sigma Chemical Co. In a typical experiment, the glycosidase (0.013 U/mL) was pre-incubated at 33 °C for 5 min in the presence of the inhibitor in 50 mM acetate buffer (pH 5.6). The reaction was started by addition of the appropriate *p*-nitrophenyl glycoside substrate (1 mM) to a final volume of 250 µl. The reaction was stopped after 15 min by addition of 350 µL of 0.4 M Na_2CO_3. The released *p*-nitrophenolate was quantified spectrometrically at 410 nm.

In cases where inhibition was greater than 95% at 1 mM concentration of inhibitor (compounds **5** and **6a**), IC_{50} values were determined after assaying decreasing concentrations of inhibitor. The inhibitory constant IC_{50} is the concentration of inhibitor causing half-maximal enzyme activity. All the assays were done in duplicate (less than 10% variability in each case).

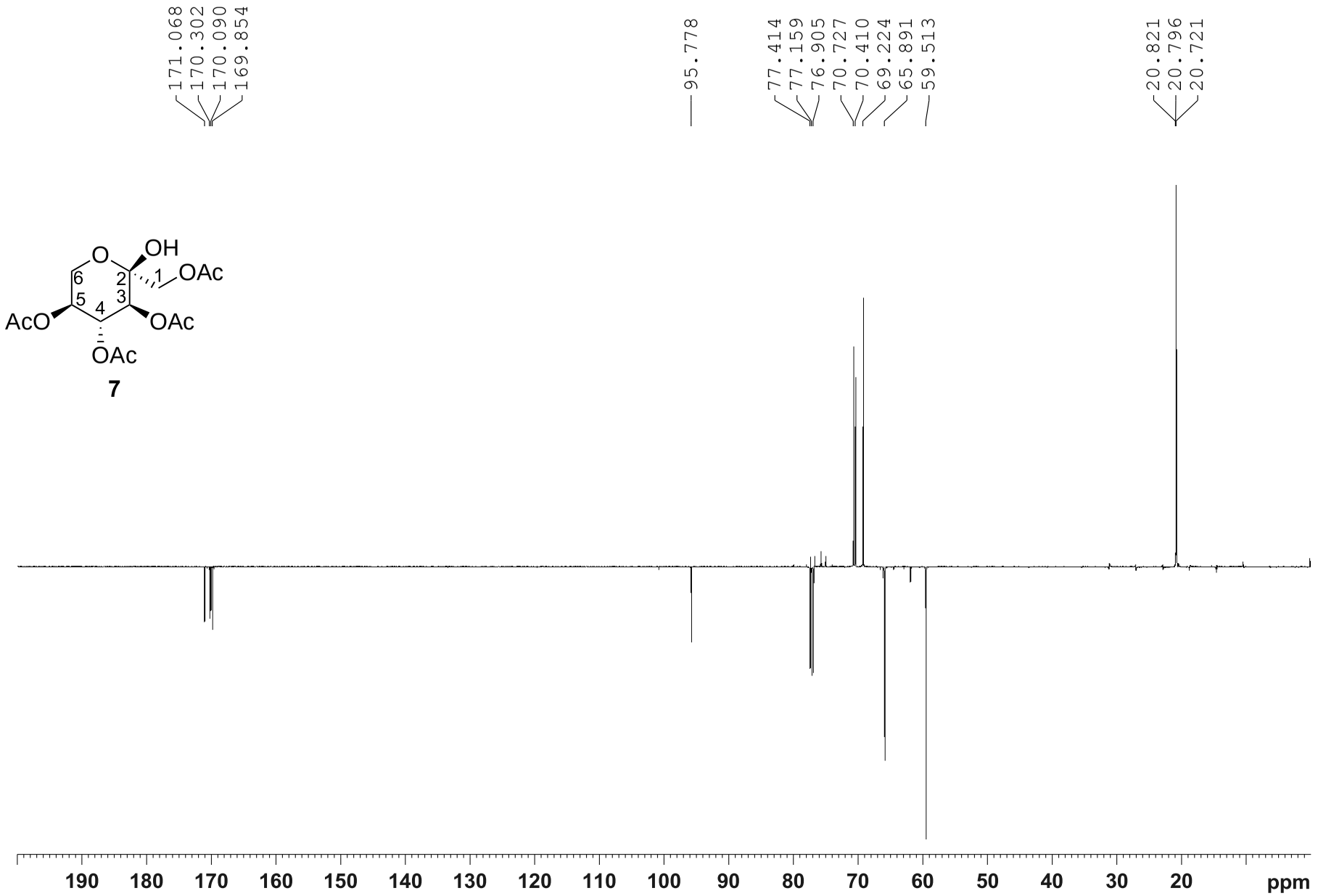
4- Copies of ^{1}H, ^{13}C and 2D NOESY spectra

^{1}H NMR ($CDCl_3$, 500 MHz)



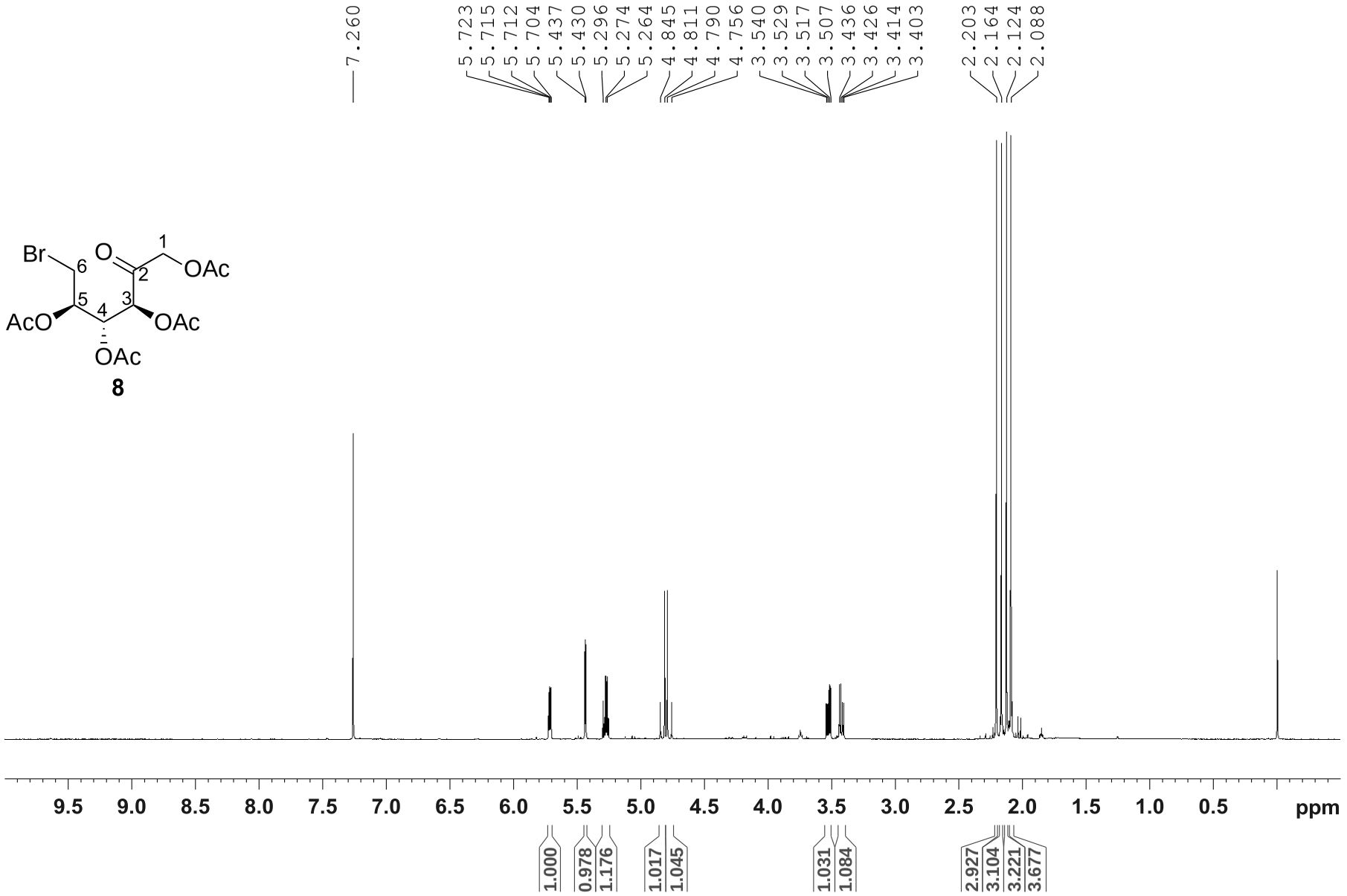
7

^{13}C NMR ($CDCl_3$, 125 MHz)

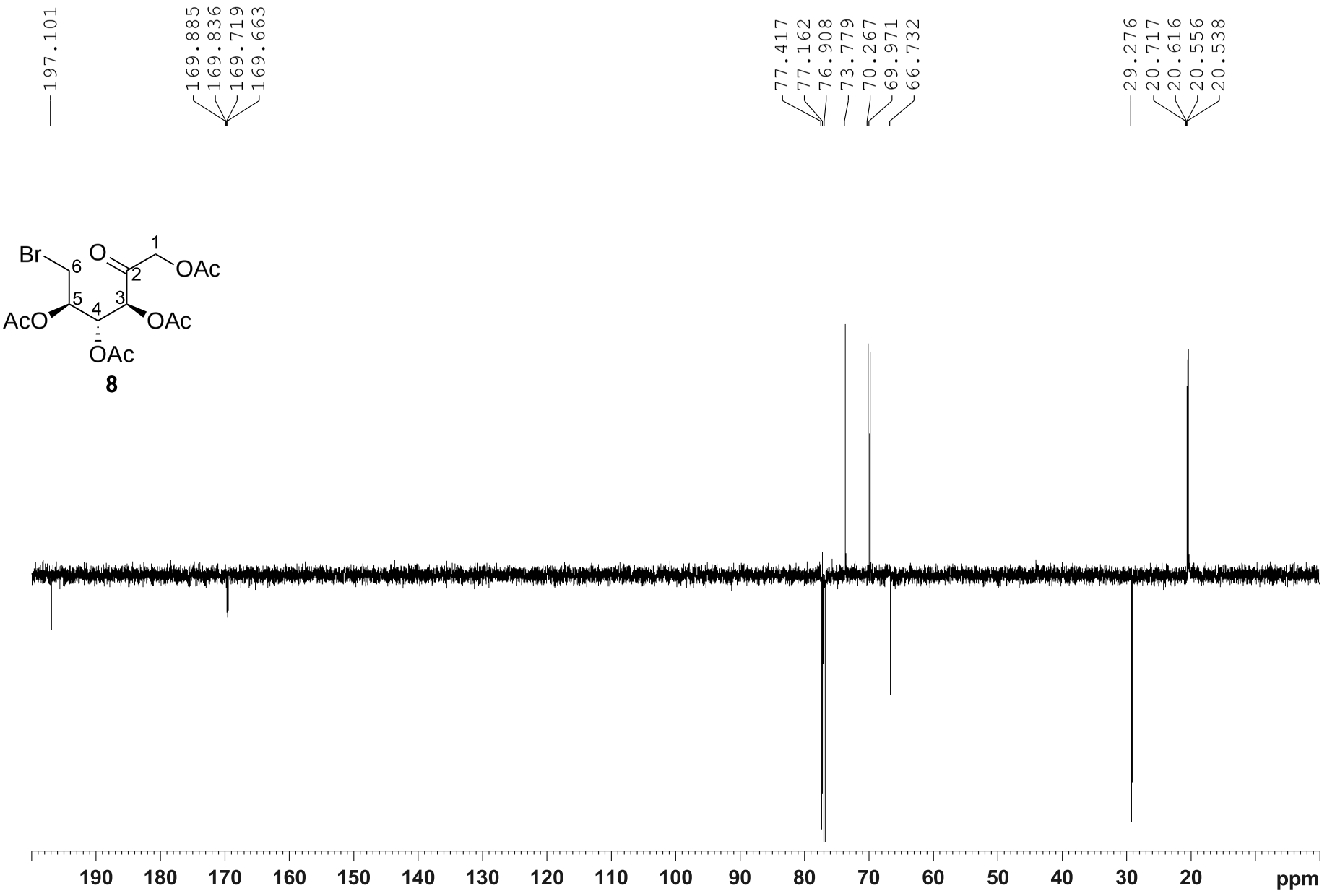


7

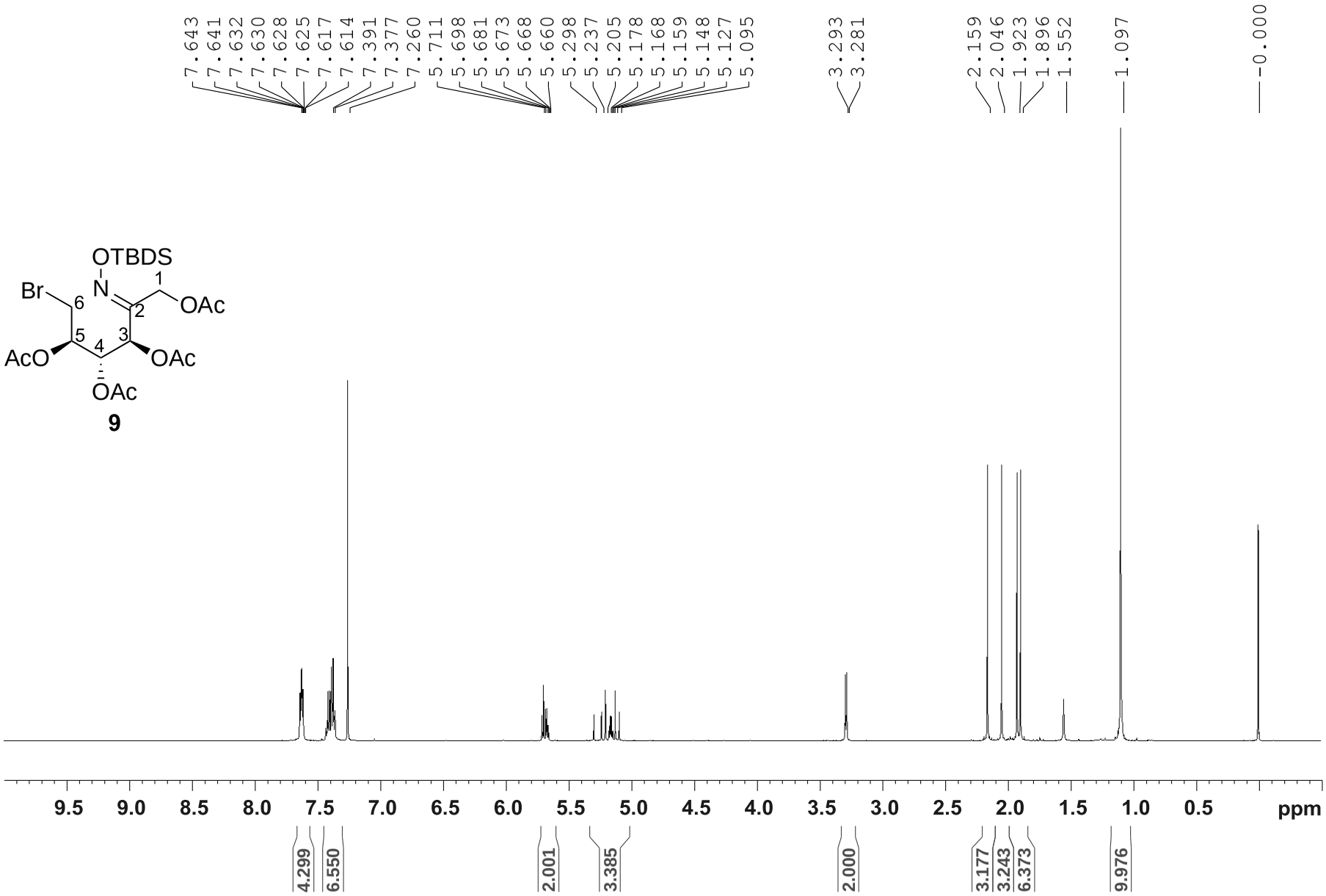
^{1}H NMR ($CDCl_3$, 500 MHz)



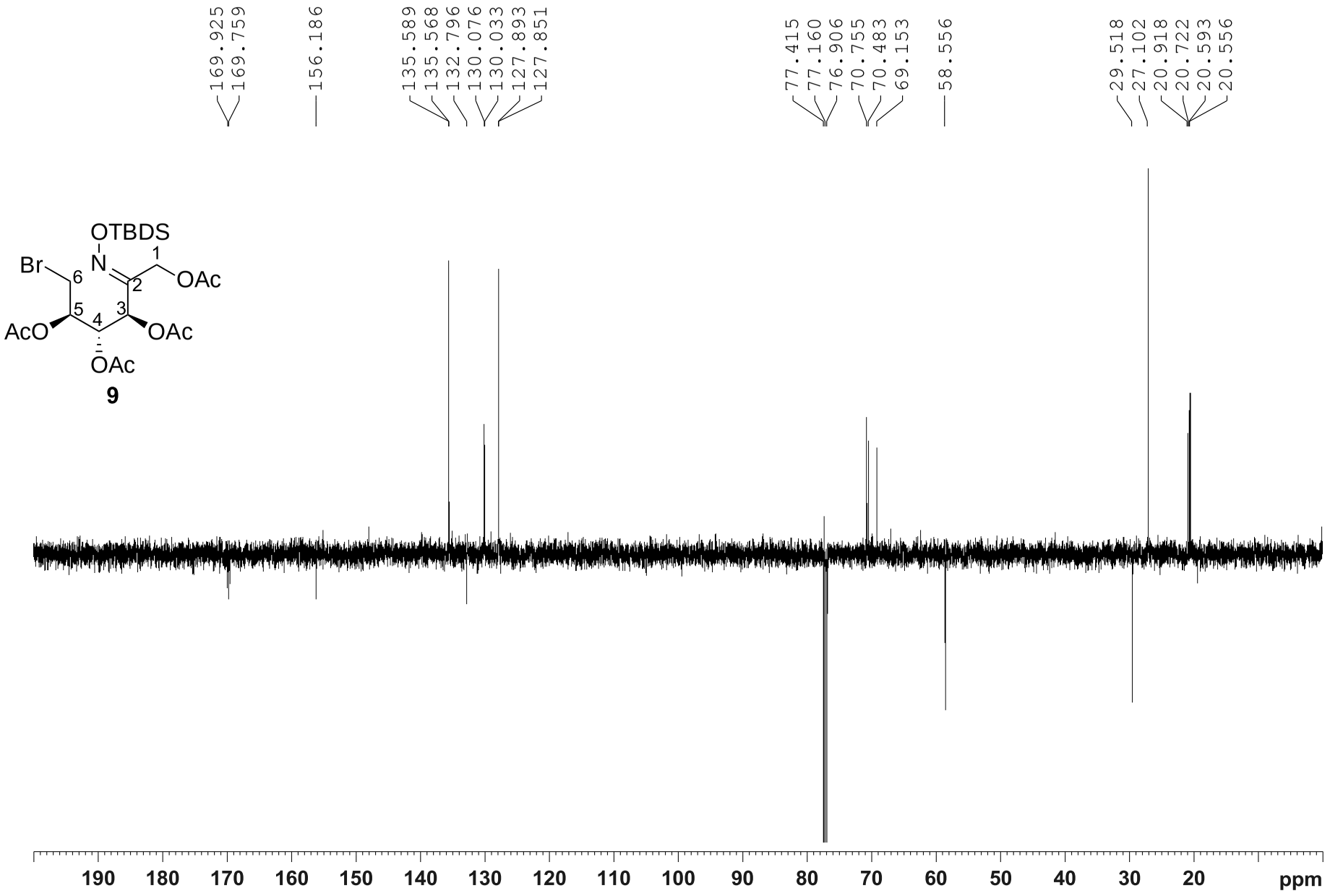
^{13}C NMR ($CDCl_3$, 125 MHz)



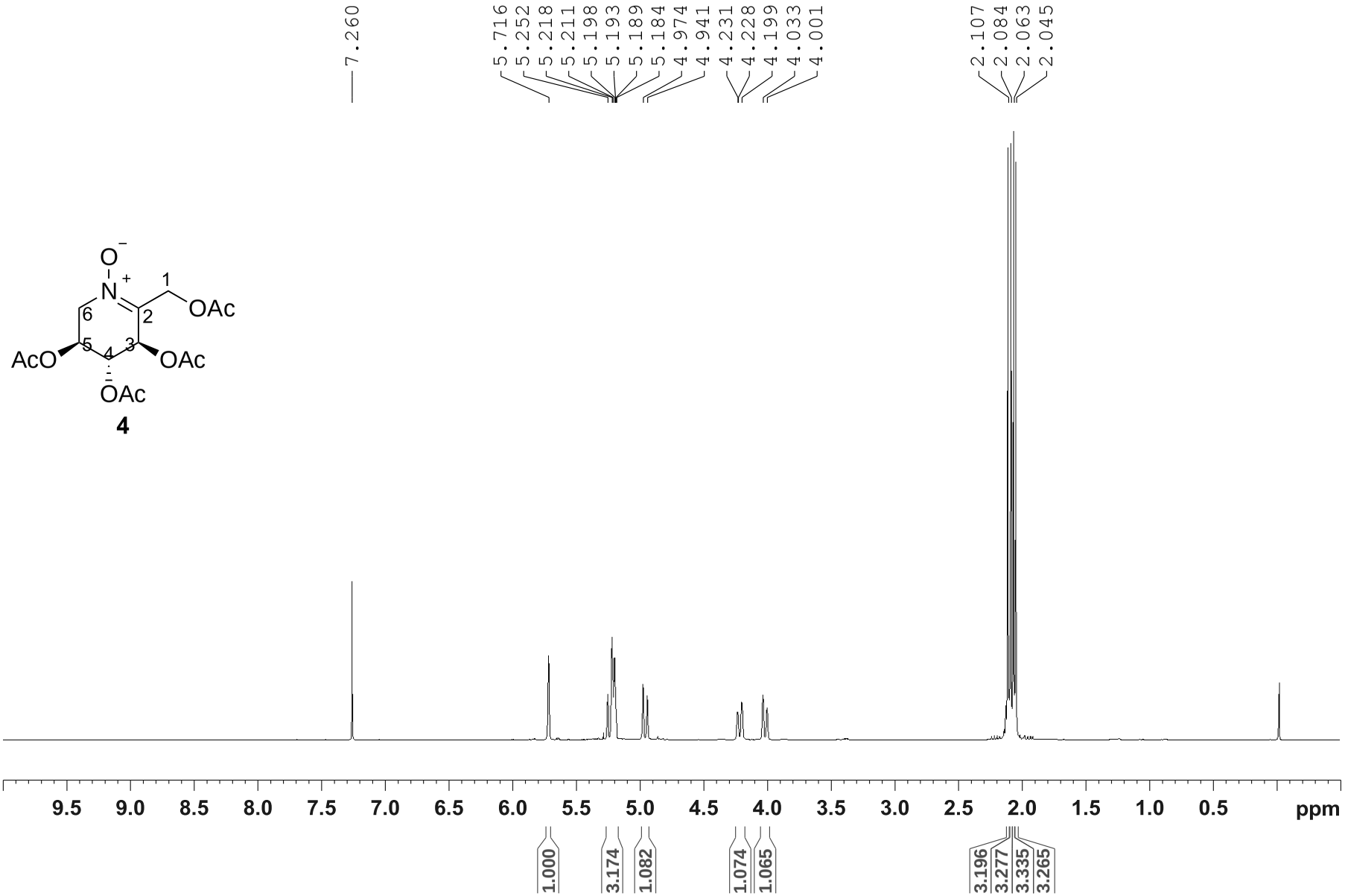
^{1}H NMR ($CDCl_3$, 500 MHz)



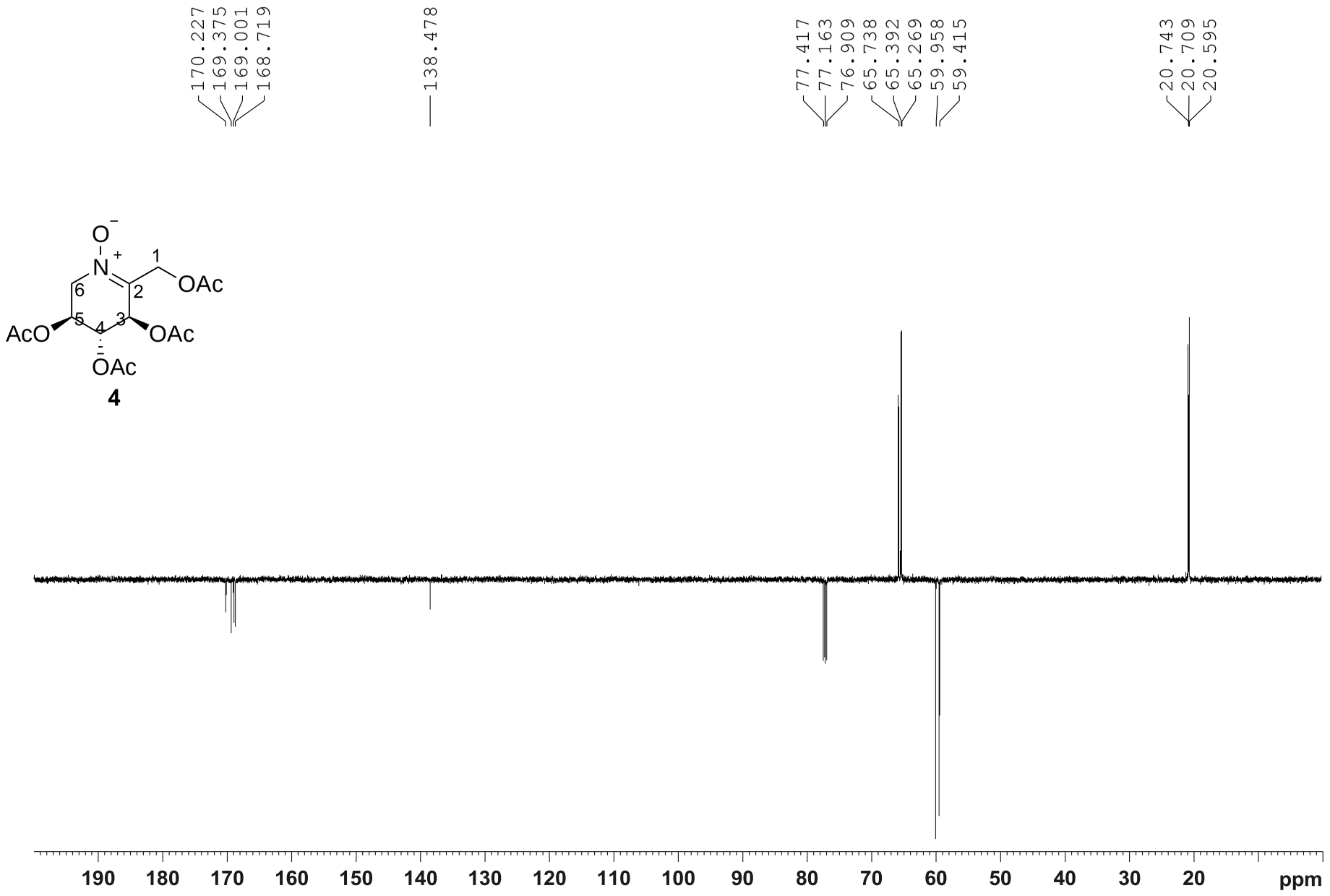
^{13}C NMR ($CDCl_3$, 125 MHz)



^{1}H NMR ($CDCl_3$, 500 MHz)

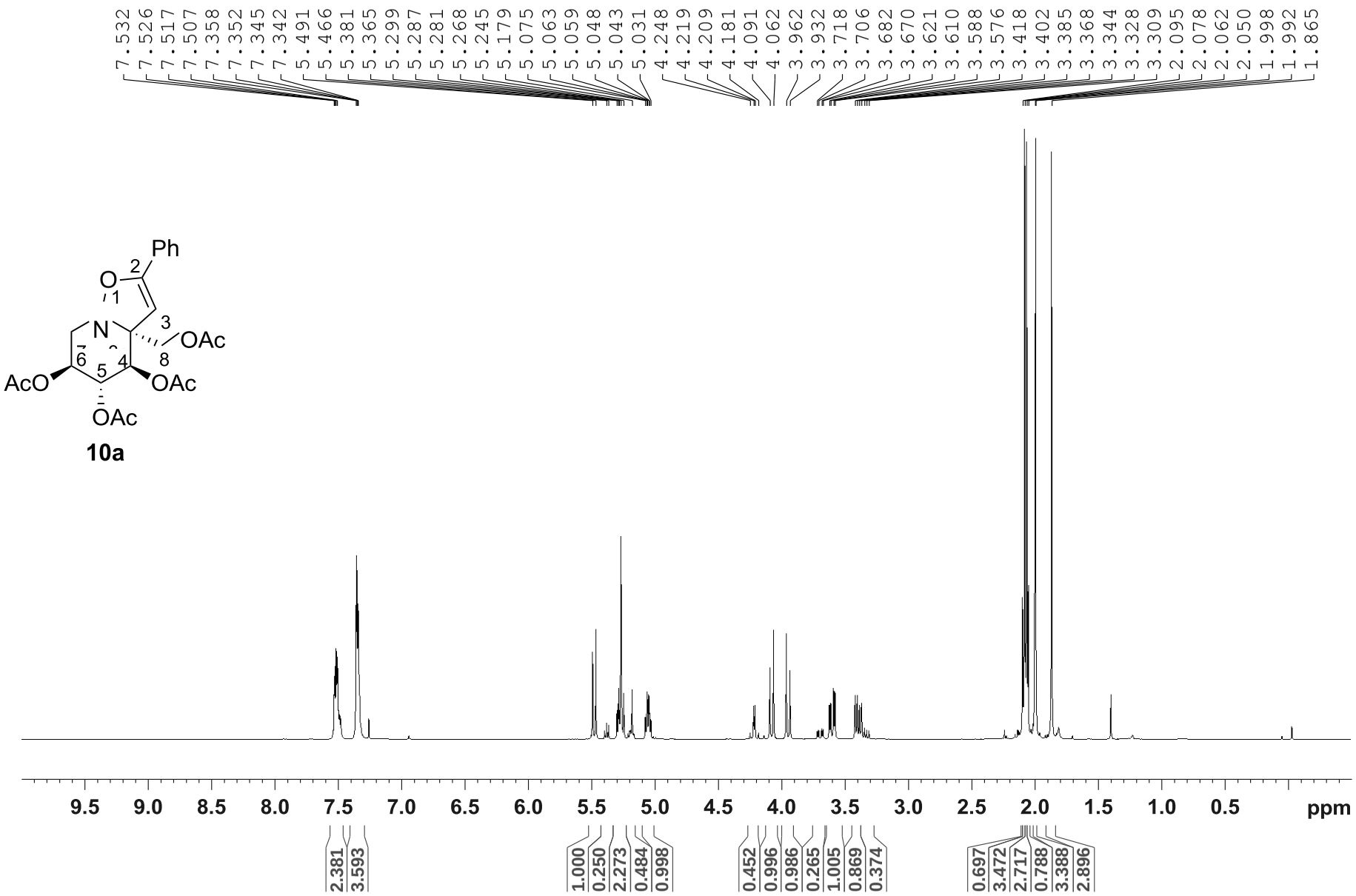


^{13}C NMR ($CDCl_3$, 125 MHz)



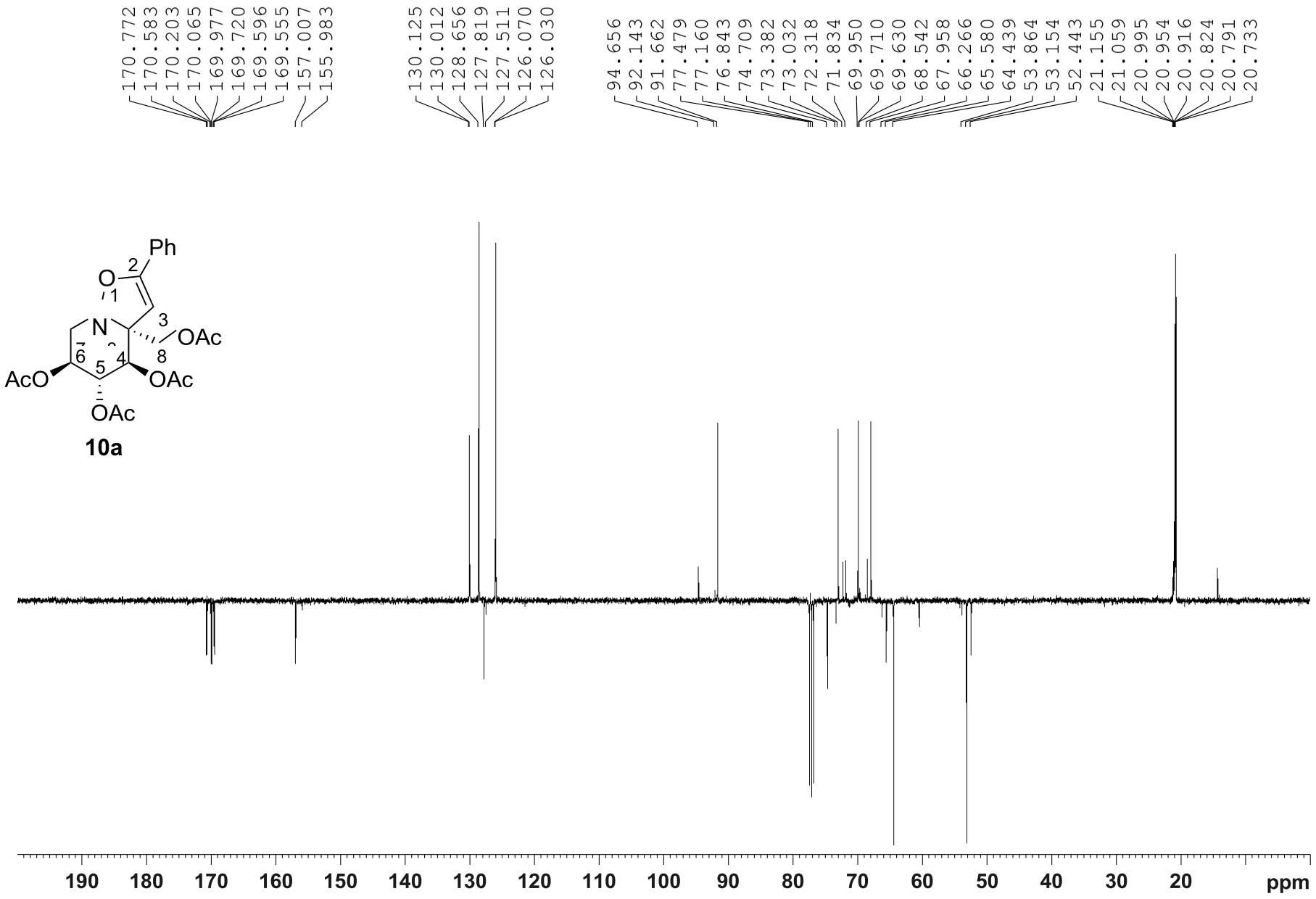
4

^{1}H NMR ($CDCl_3$, 400 MHz)



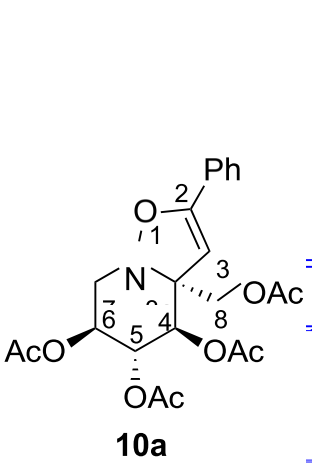
10a

^{13}C NMR ($CDCl_3$, 100 MHz)

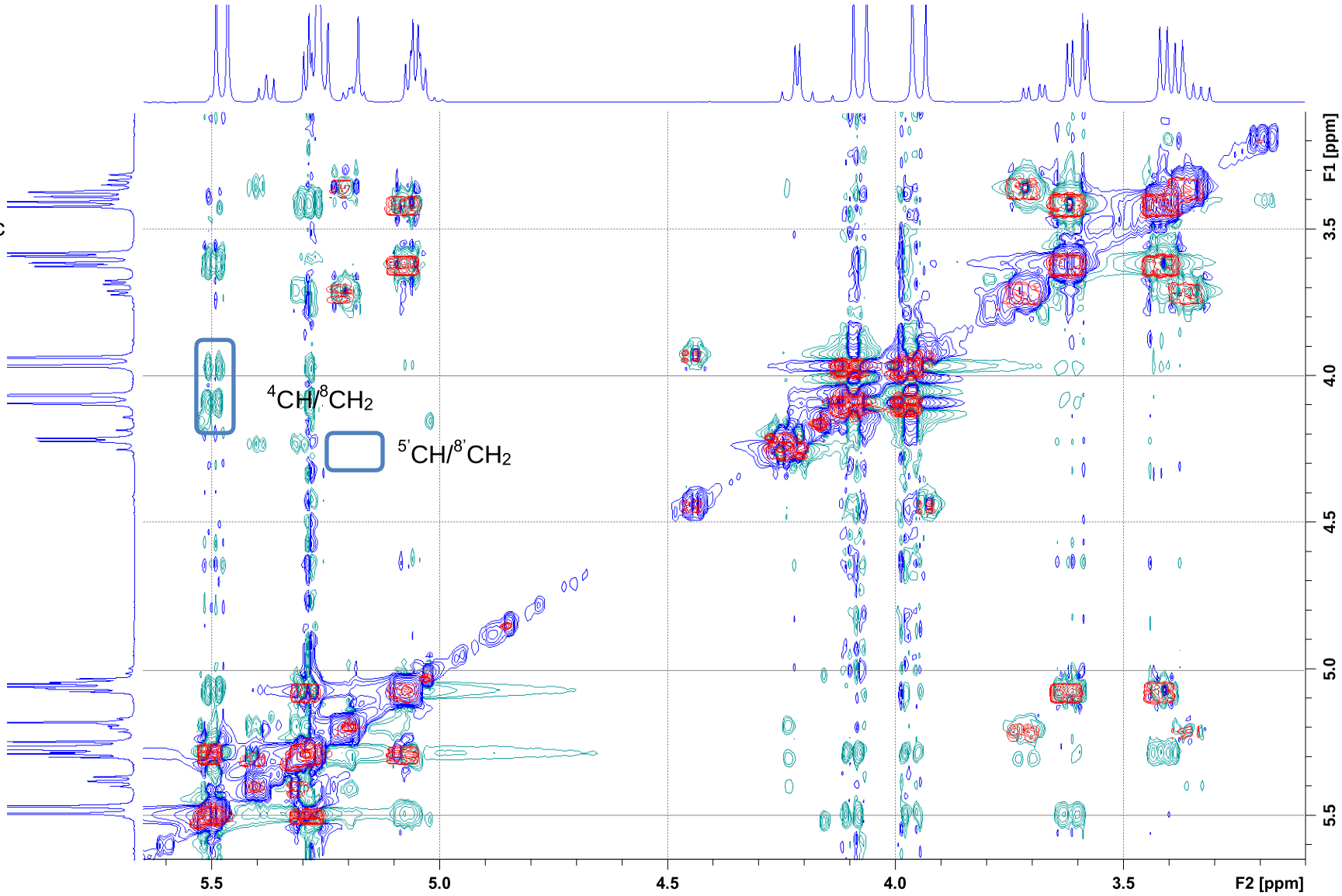


10a

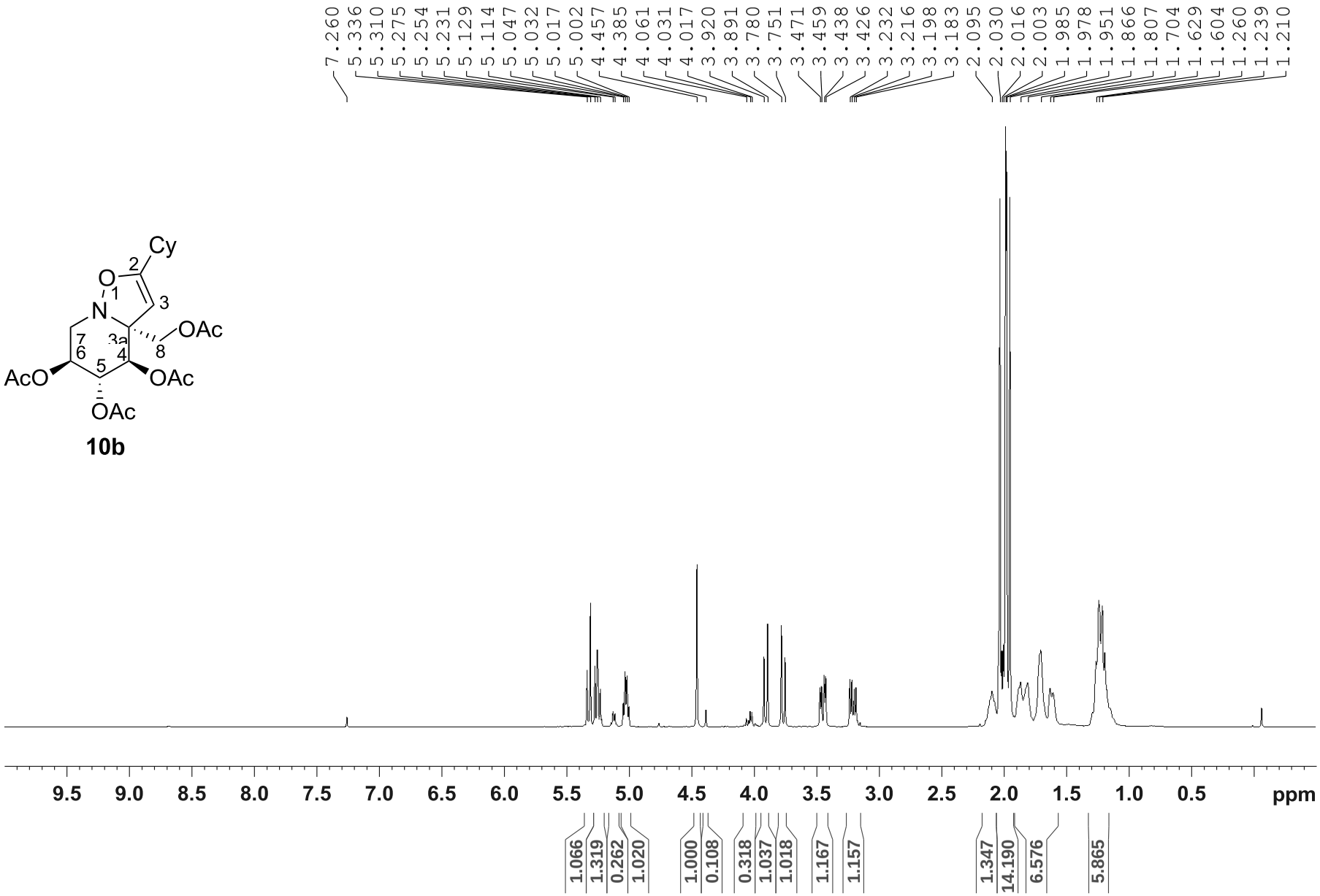
NOESY (green), COSY (red) correlations ($CDCl_3$, 400 MHz)



10a

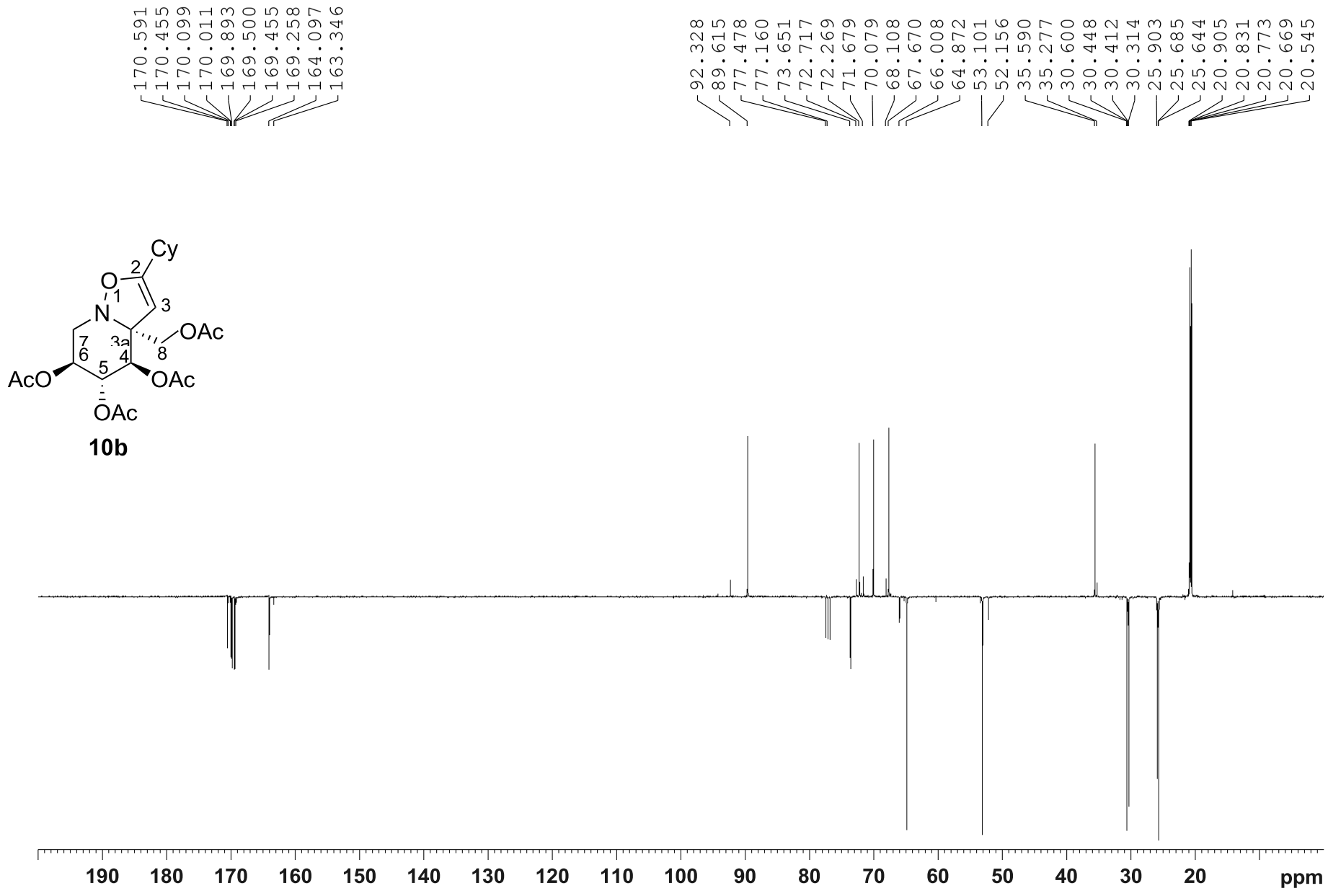


^{1}H NMR ($CDCl_3$, 400 MHz)



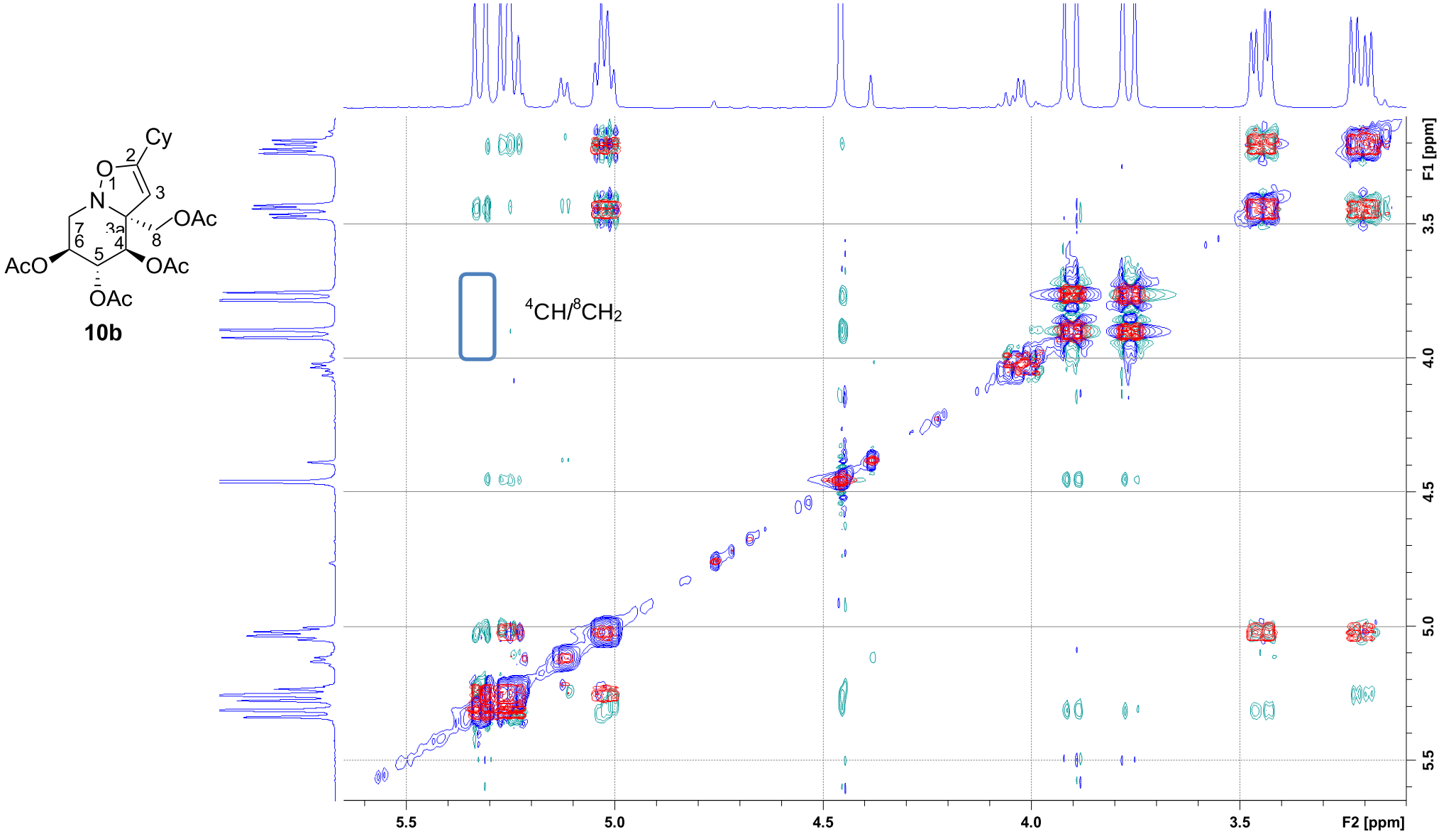
10b

^{13}C NMR ($CDCl_3$, 100 MHz)

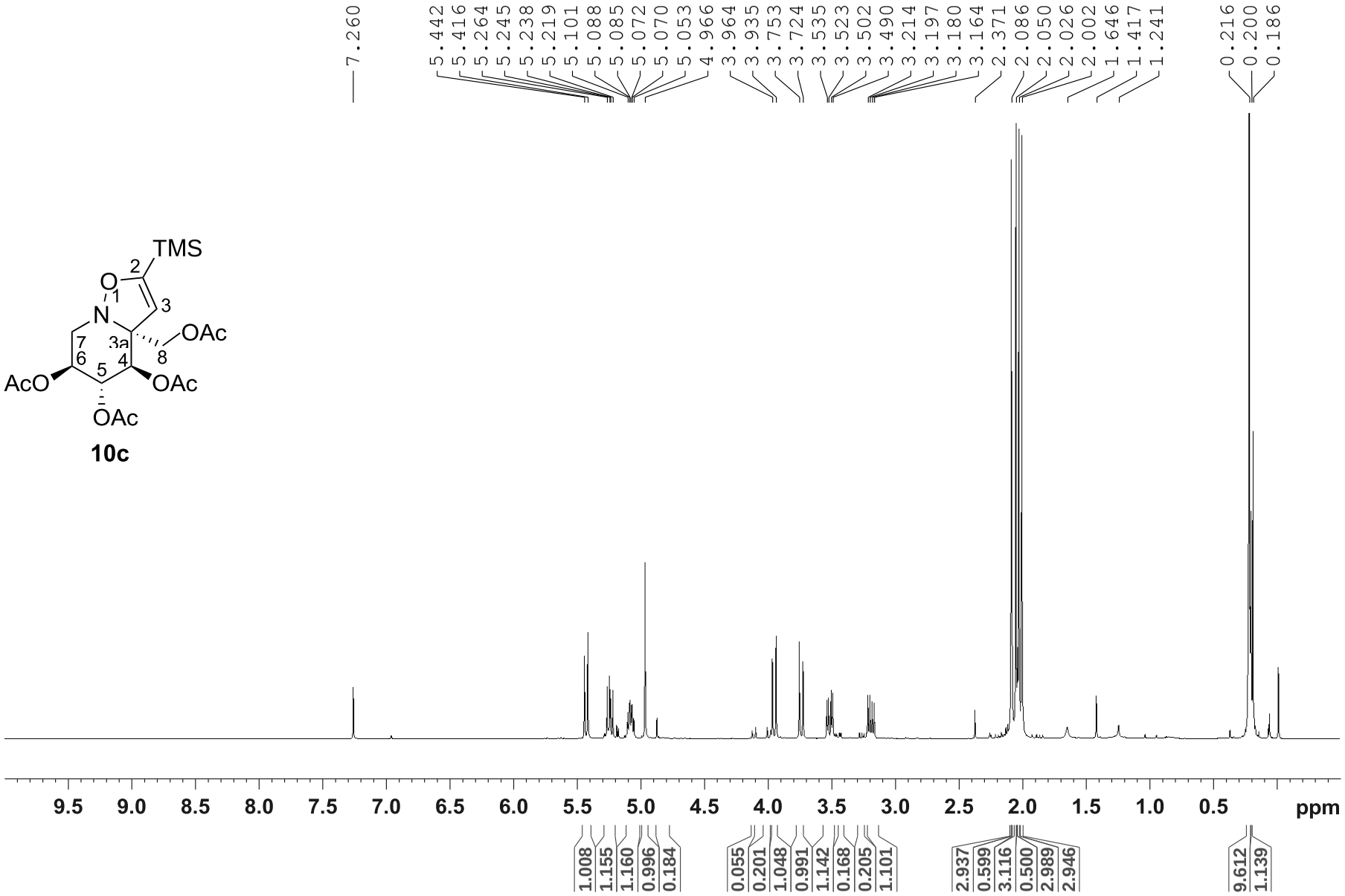


10b

NOESY (green), COSY (red) correlations ($CDCl_3$, 400 MHz)

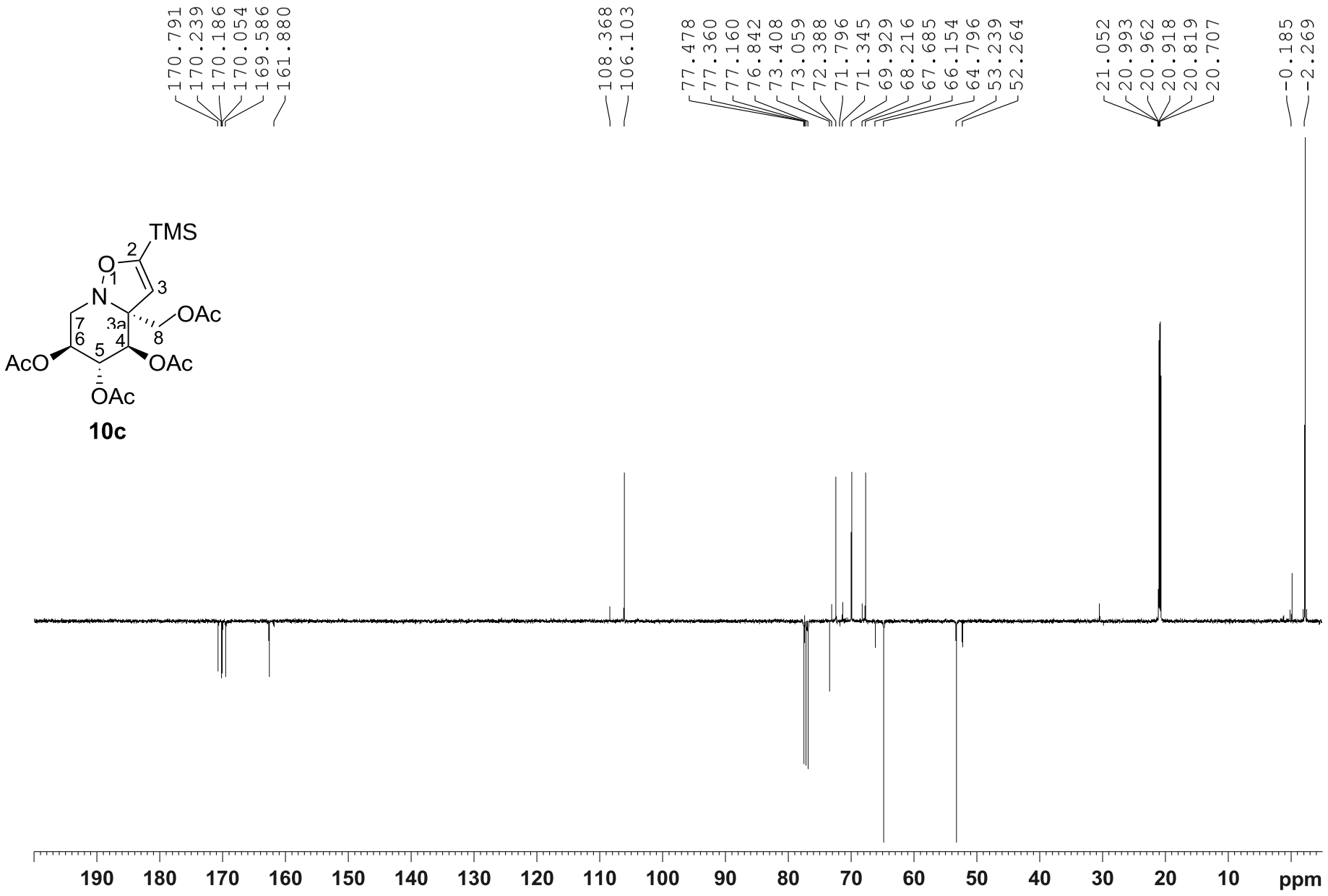


^{1}H NMR ($CDCl_3$, 400 MHz)



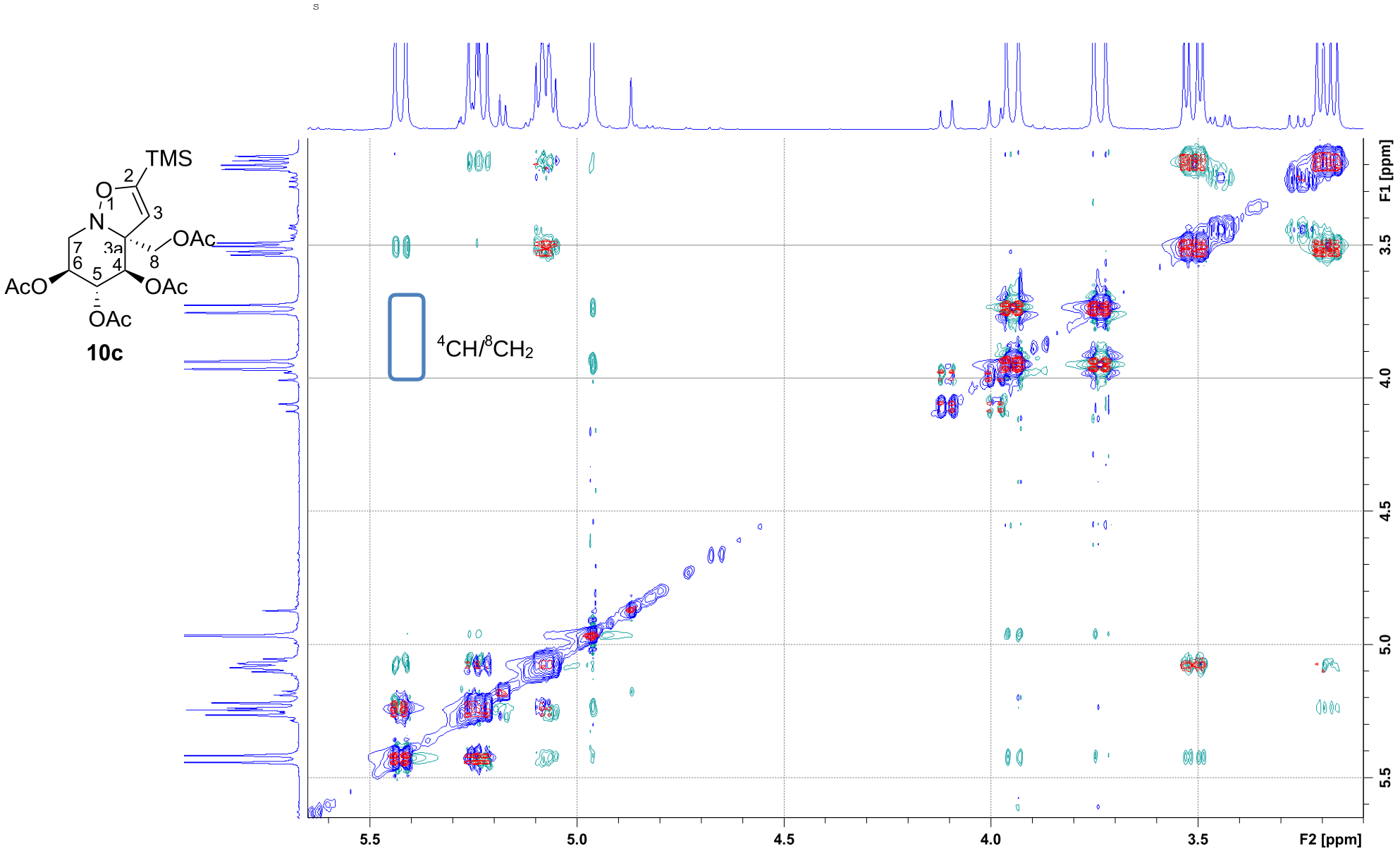
10c

^{13}C NMR ($CDCl_3$, 100 MHz)

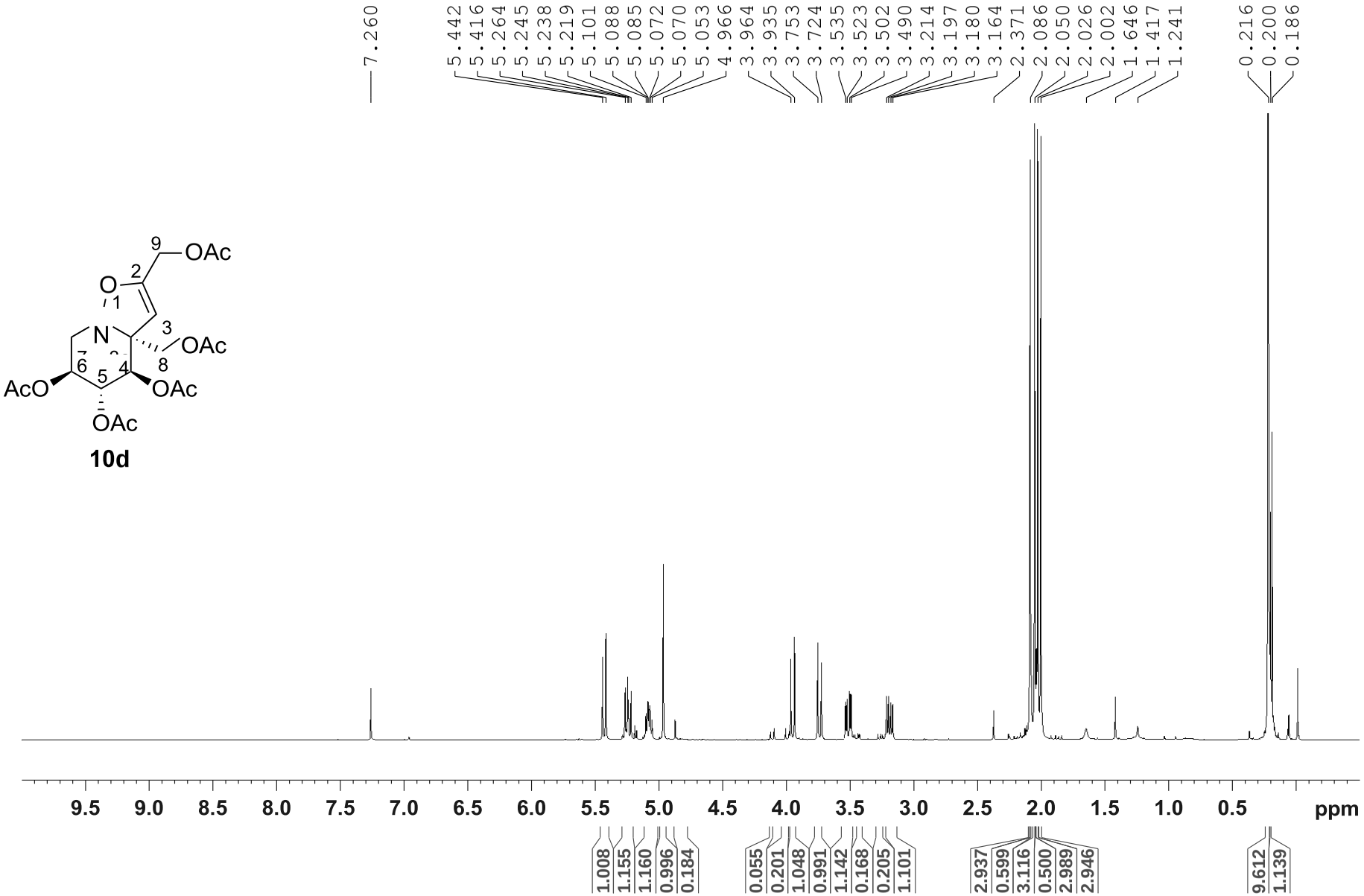


10c

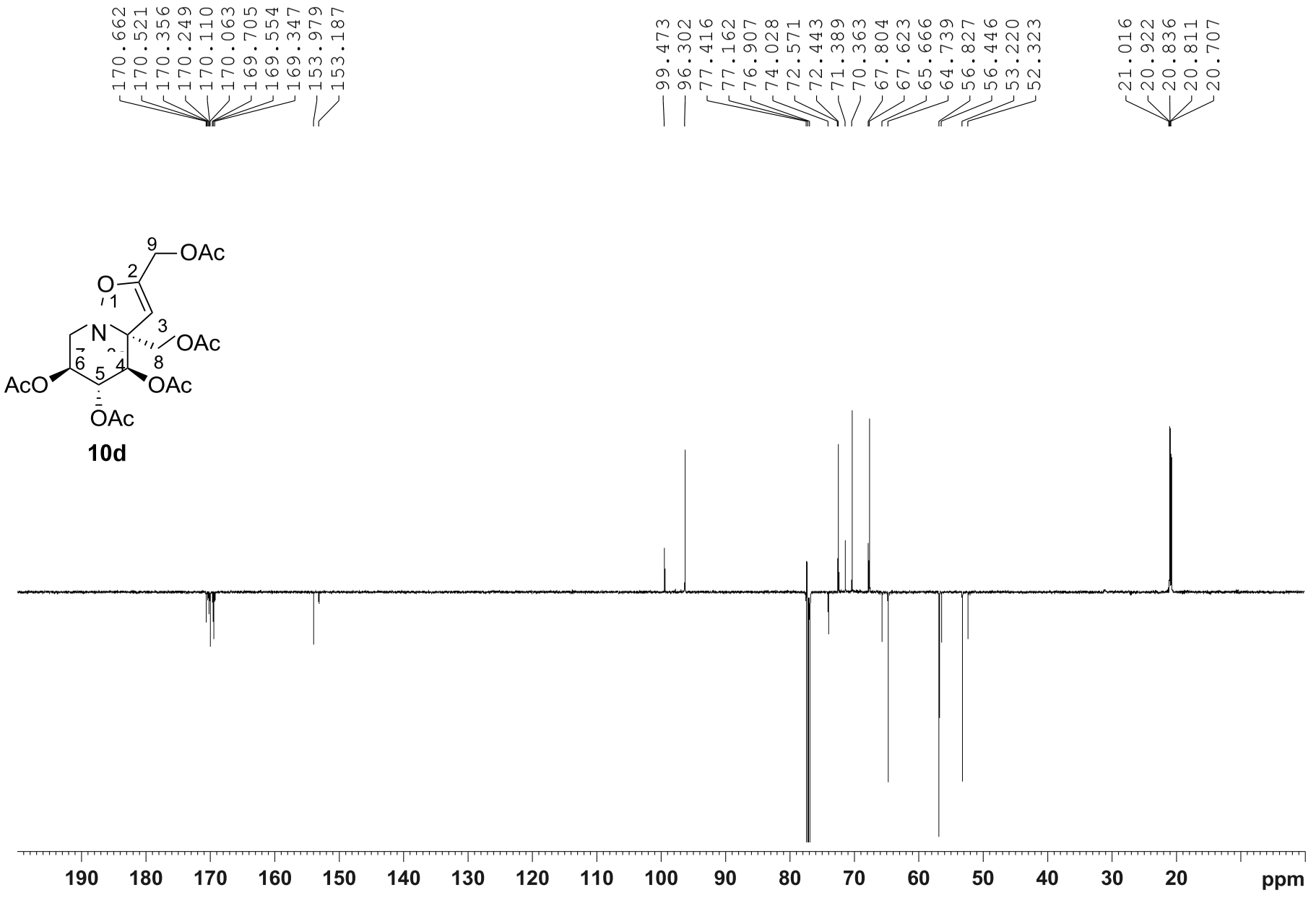
NOESY (green), COSY (red) correlations ($CDCl_3$, 400 MHz)



^{1}H NMR ($CDCl_3$, 500 MHz)

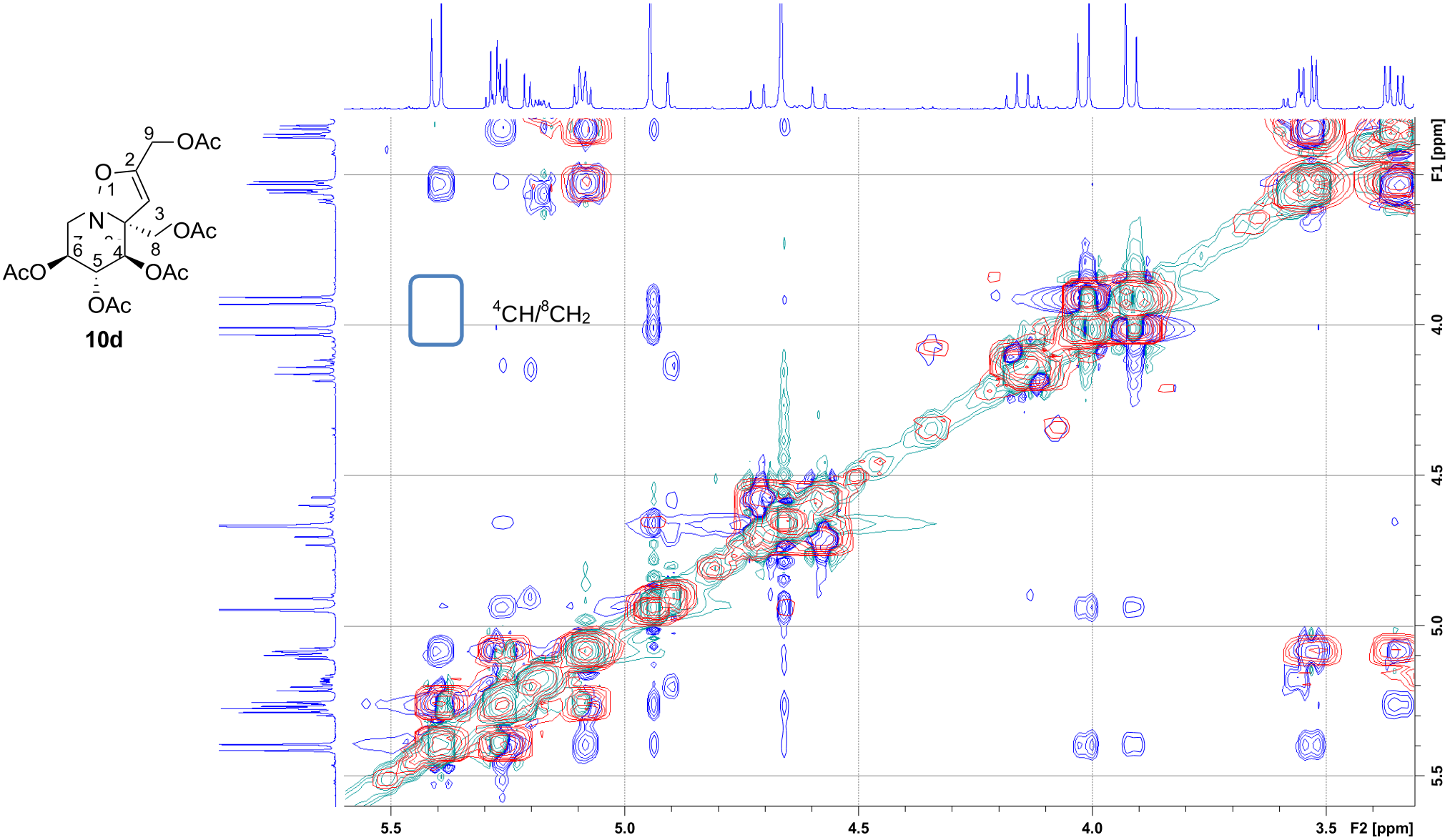


^{13}C NMR ($CDCl_3$, 125 MHz)

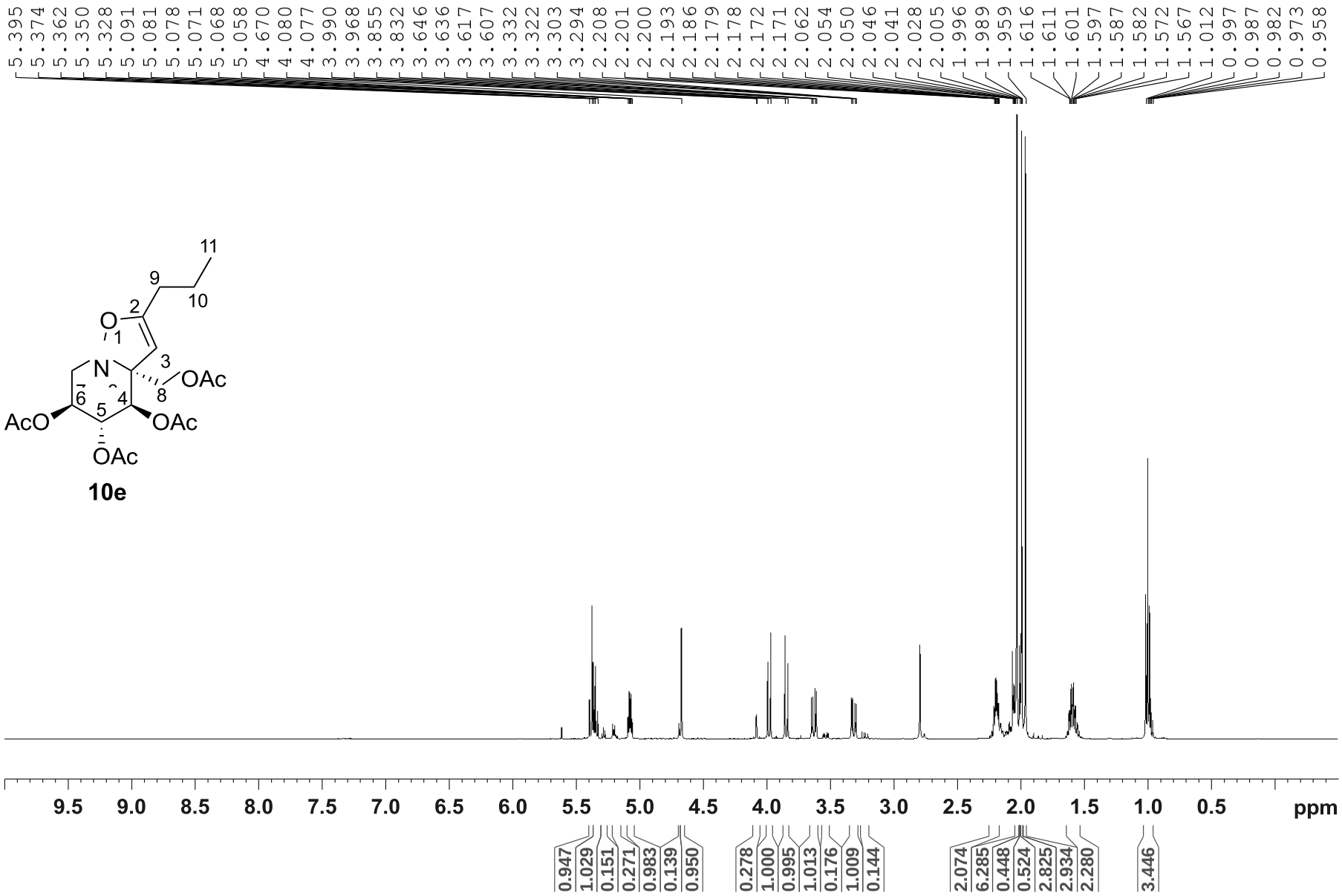


10d

NOESY (blue), COSY (red) correlations ($CDCl_3$, 500 MHz)

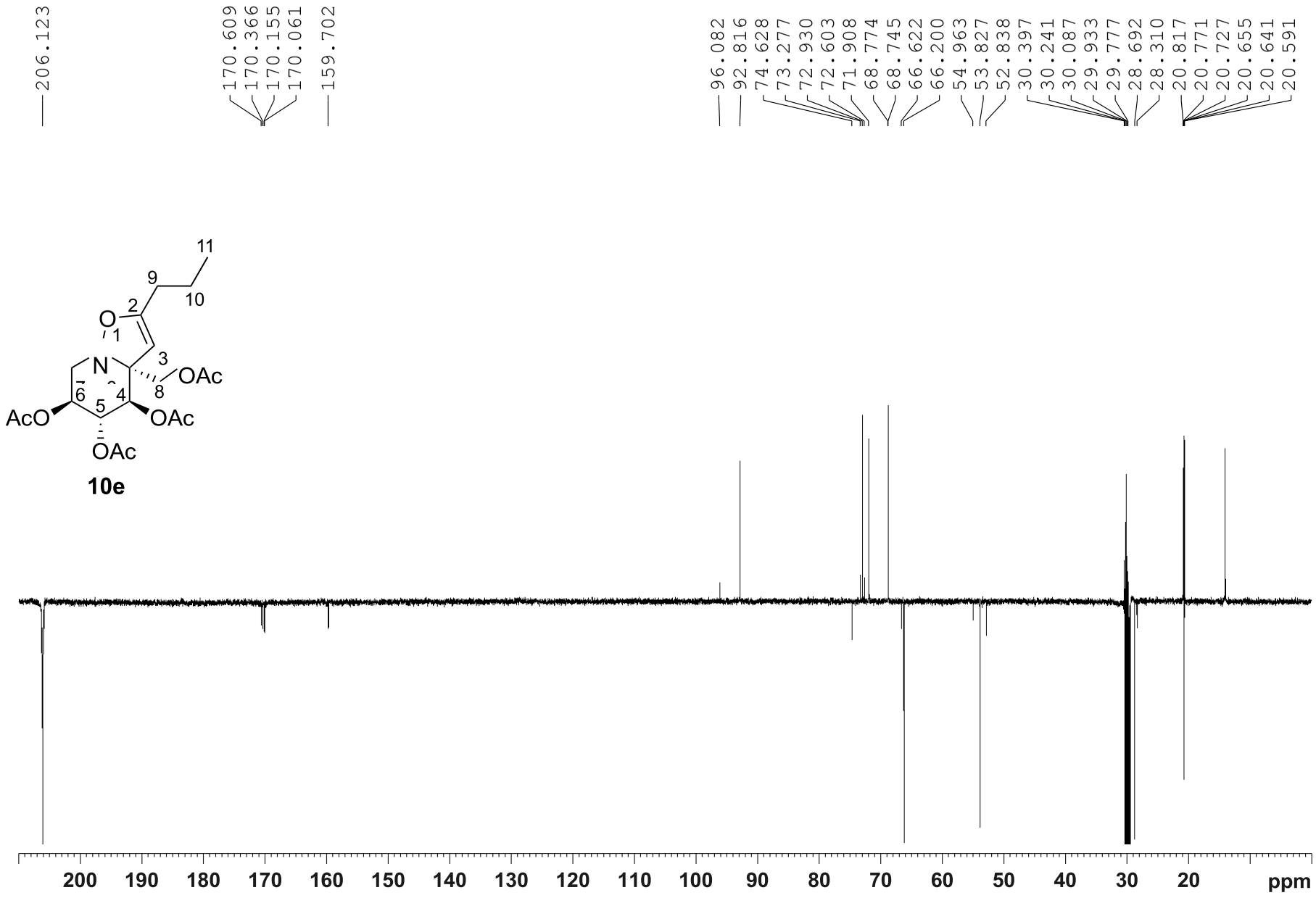


^{1}H NMR ((CD$_3$)$_2$CO, 500 MHz)



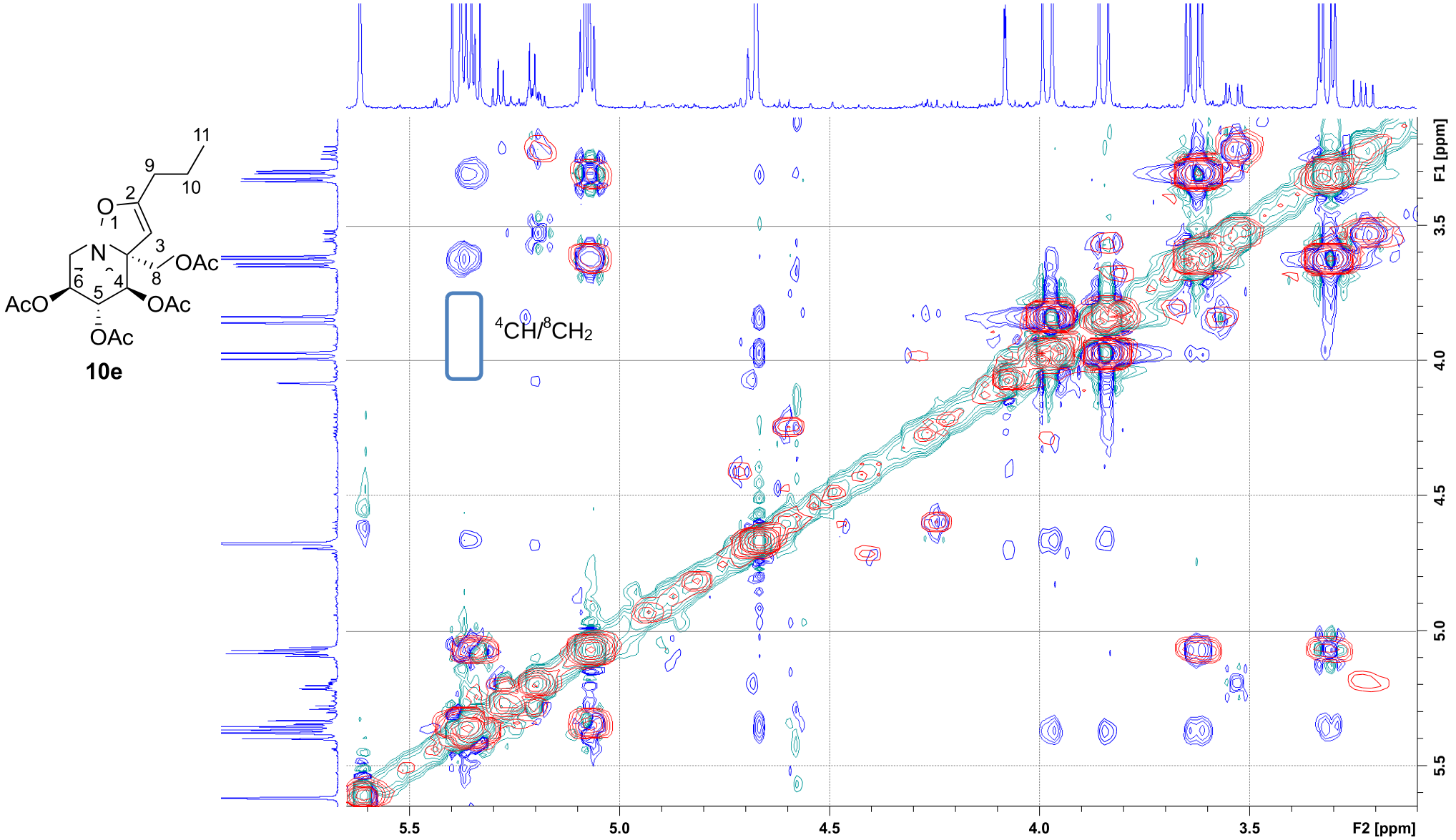
10e

^{13}C NMR ((CD$_3$)$_2$CO, 125 MHz)

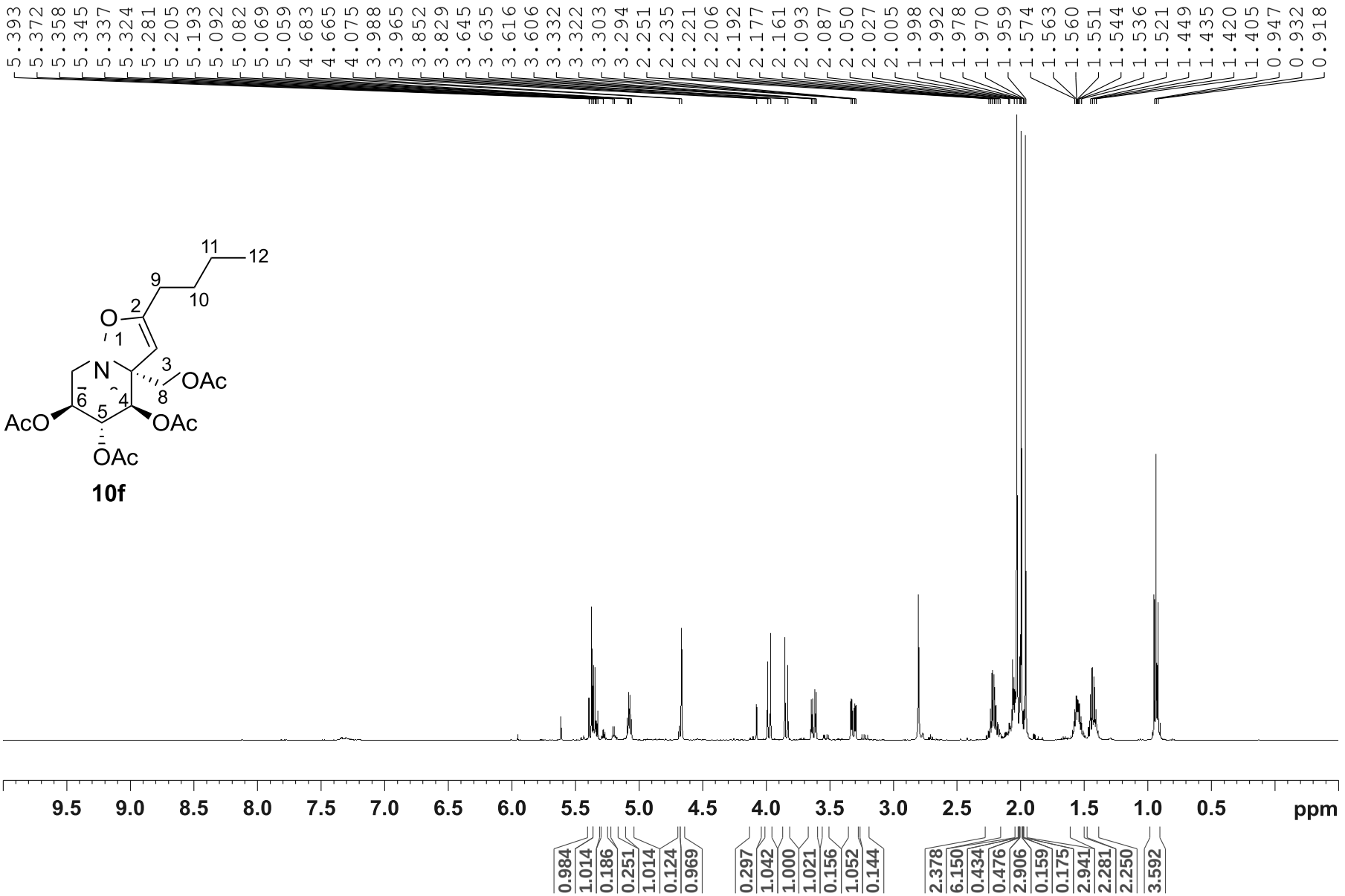


10e

NOESY (blue), COSY (red) correlations ($(CD_3)_2CO$, 500 MHz)

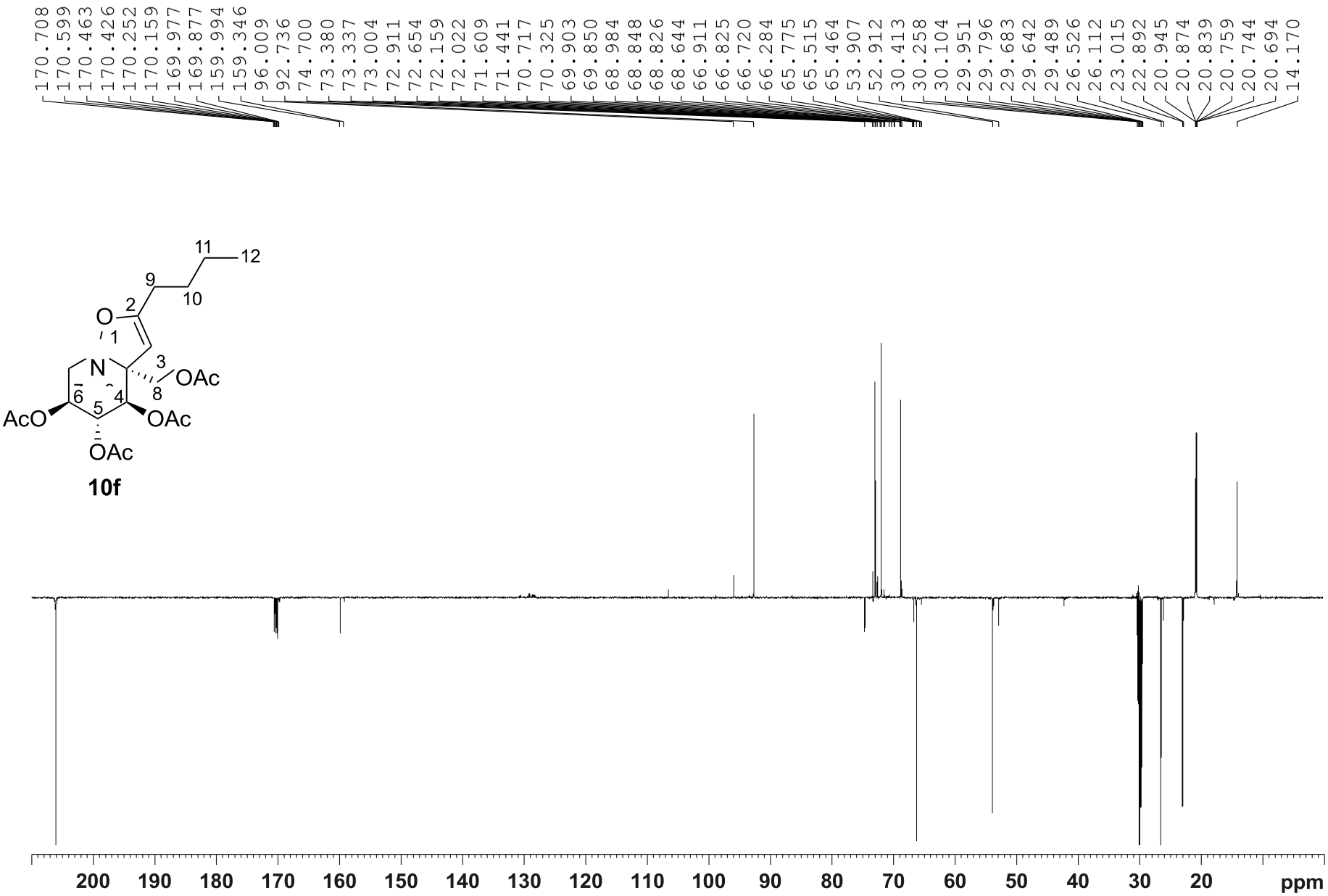


^{1}H NMR ((CD$_3$)$_2$CO, 500 MHz)

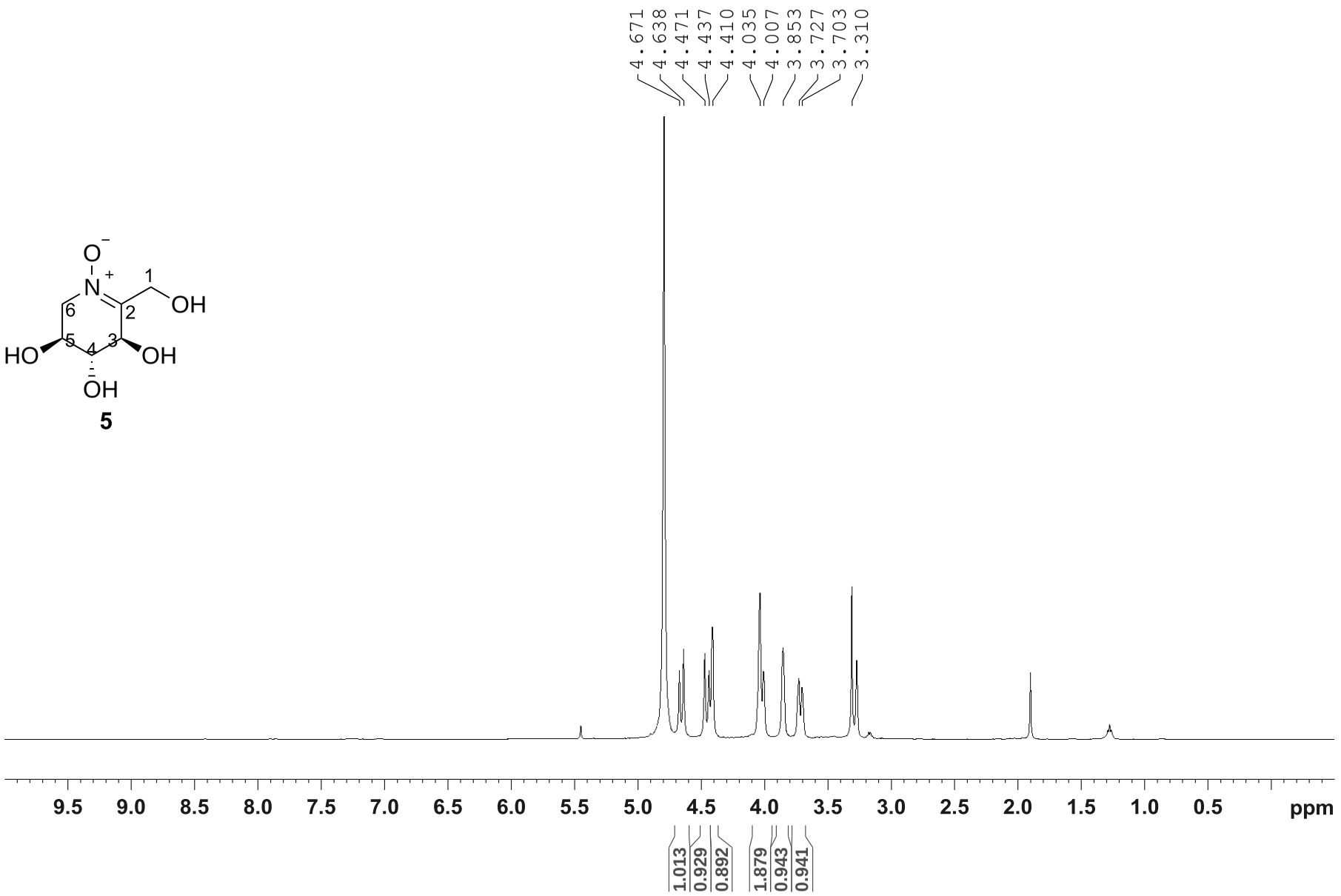


10f

^{13}C NMR ((CD$_3$)$_2$CO, 125 MHz)

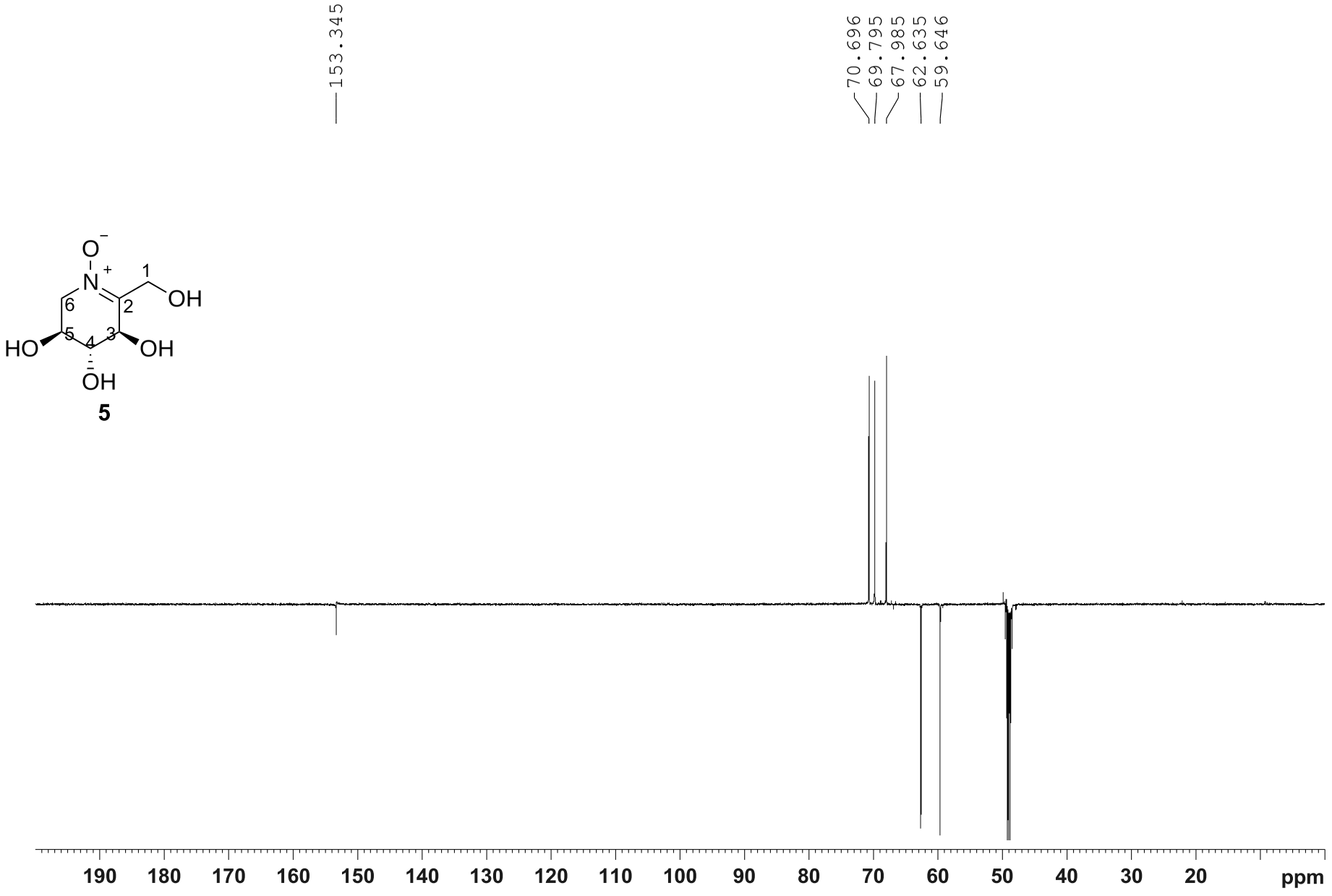


^{1}H NMR (CD_3OD, 500 MHz)



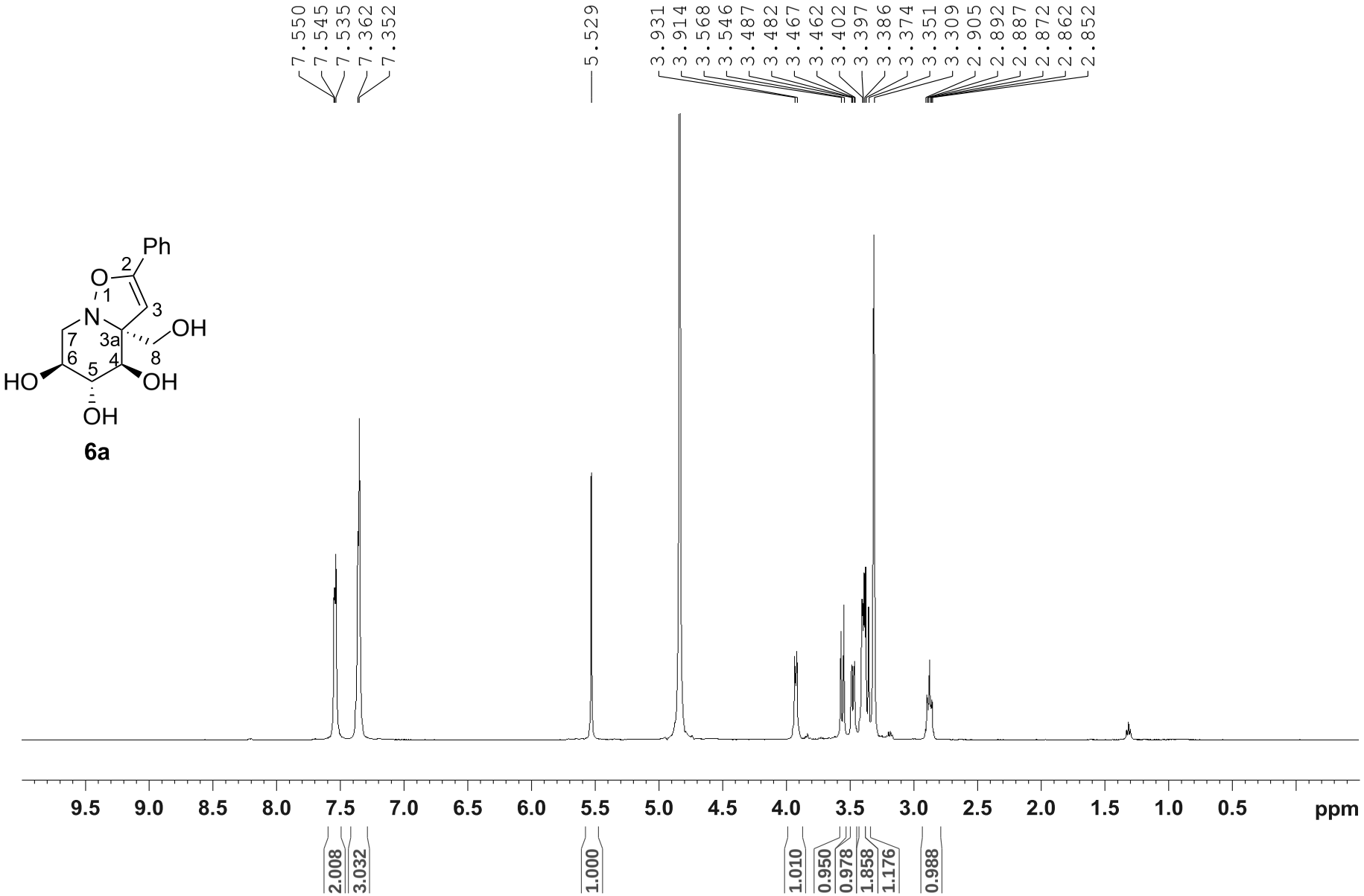
5

^{13}C NMR (CD_3OD, 125 MHz)



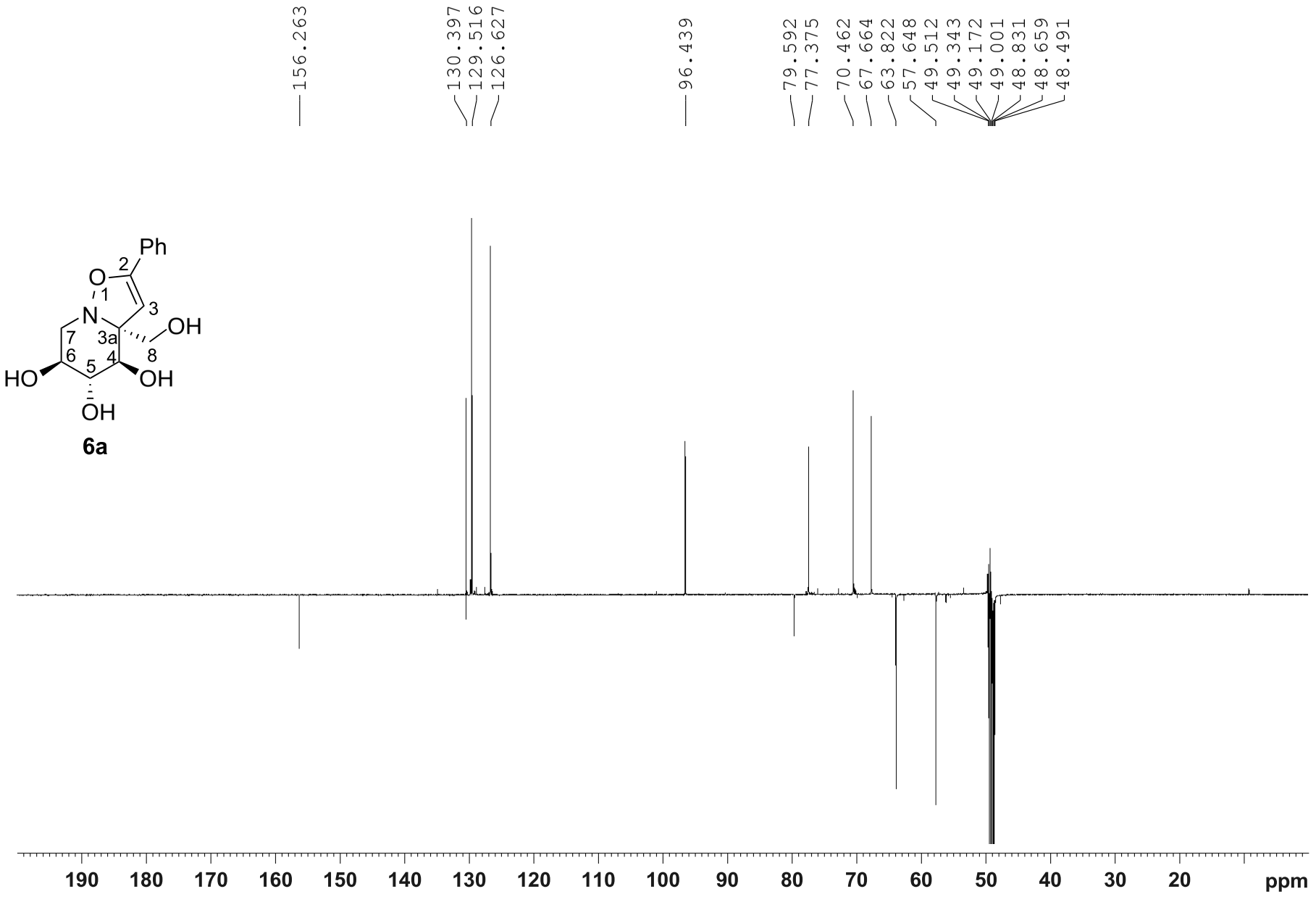
5

^{1}H NMR (CD_3OD, 500 MHz)

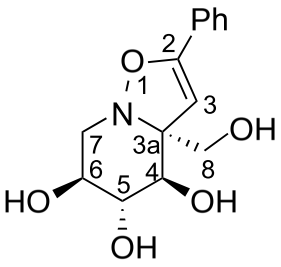


6a

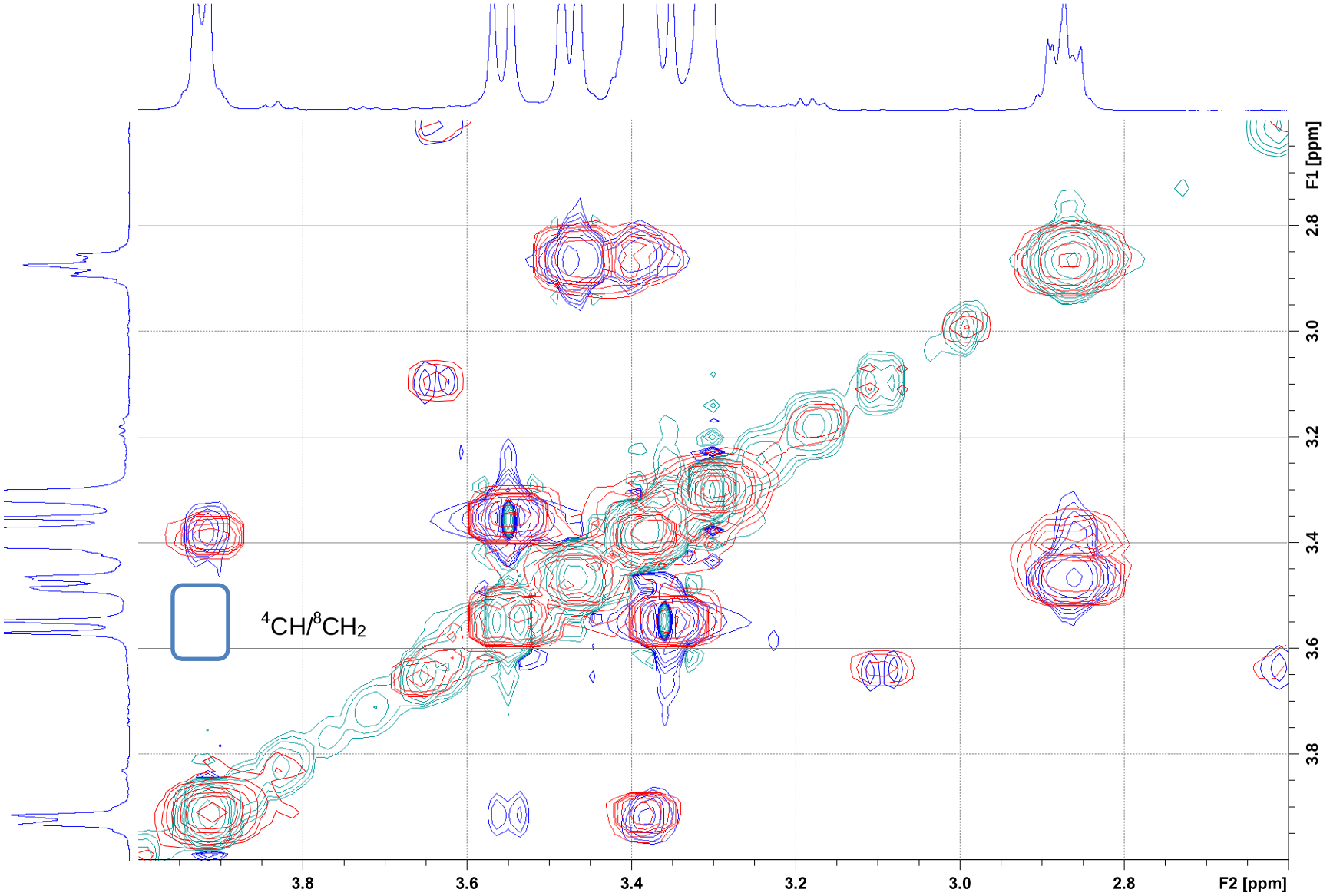
^{13}C NMR (CD_3OD, 125 MHz)



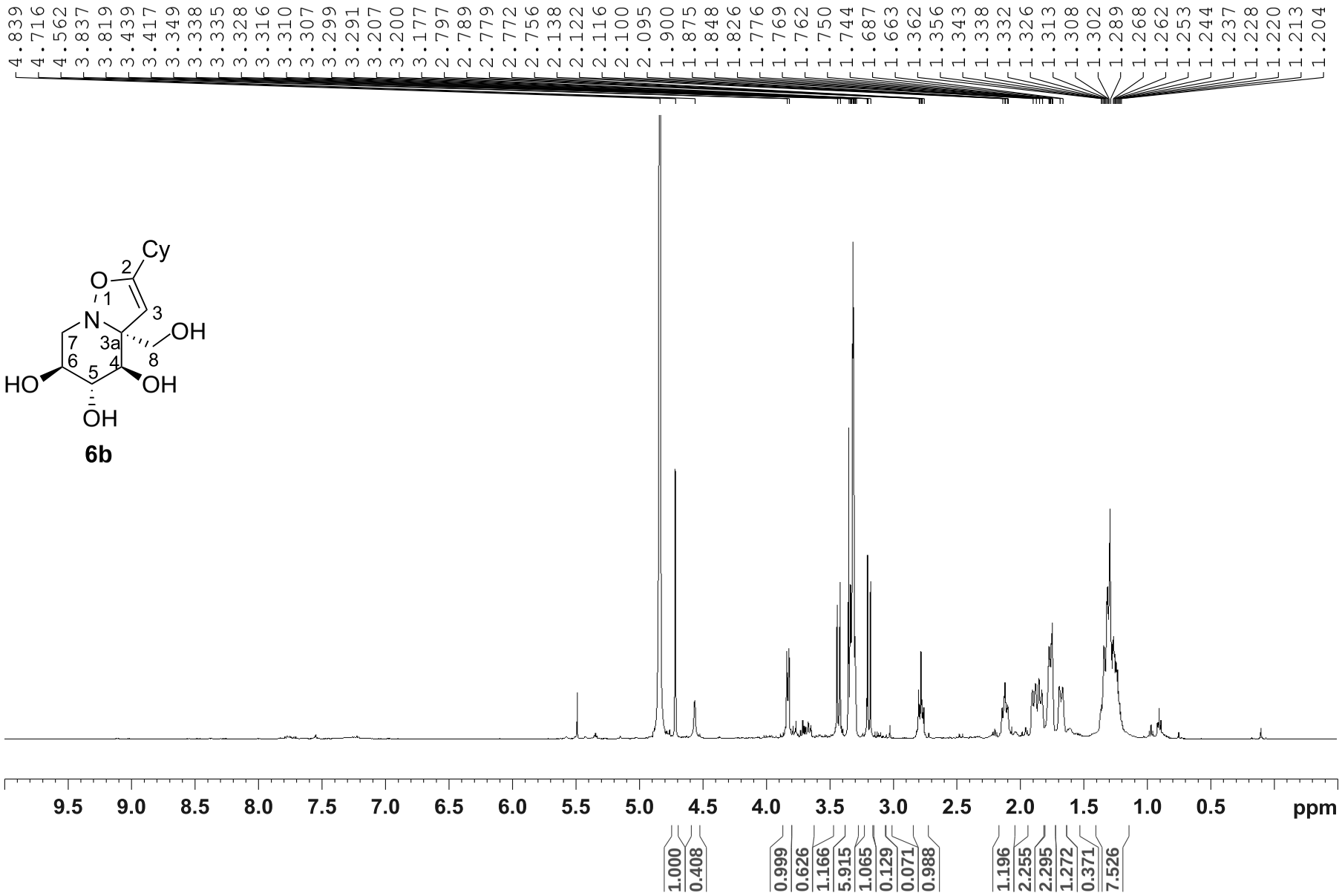
NOESY (blue), COSY (red) correlations (CD_3OD, 500 MHz)



6a

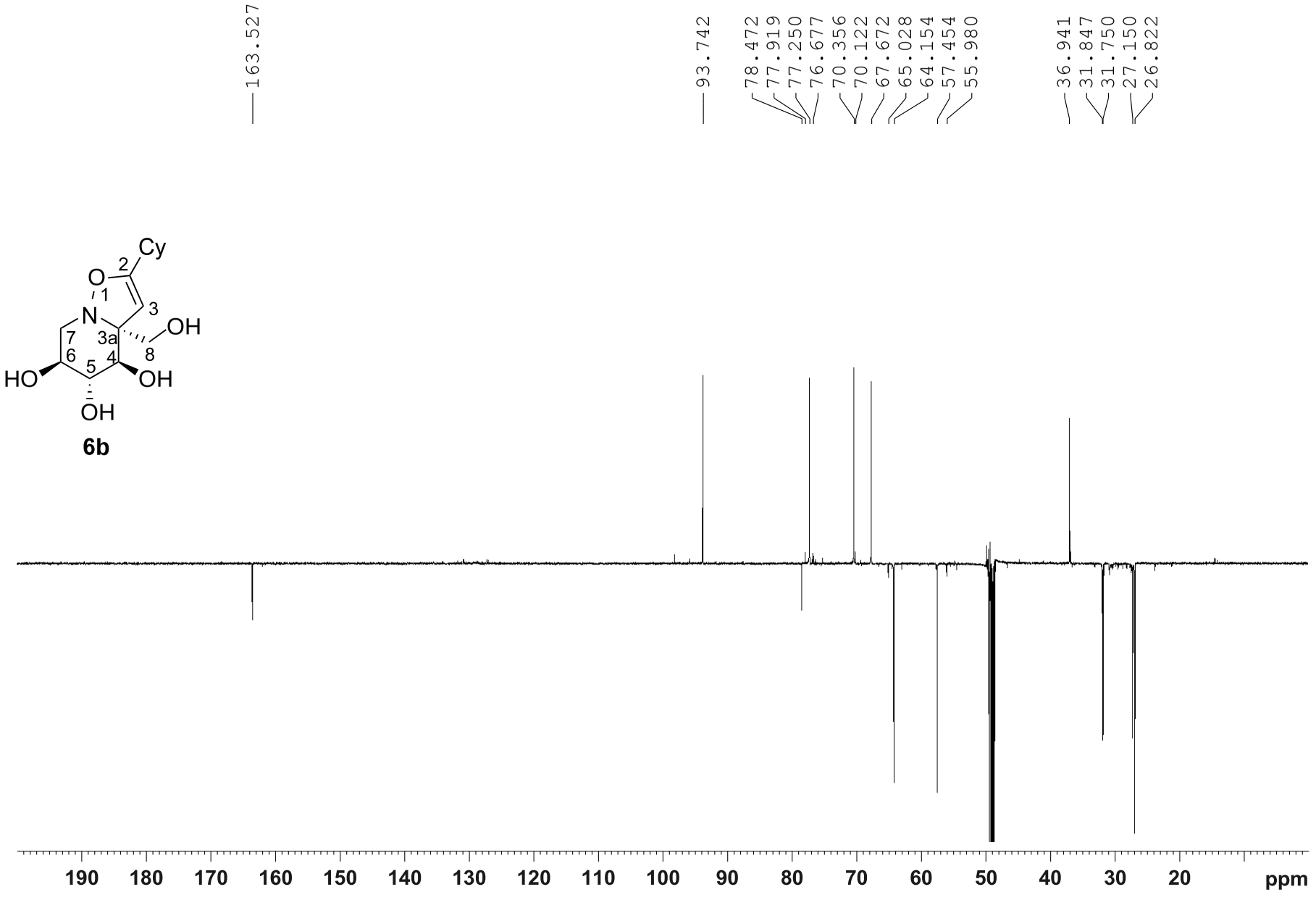


^{1}H NMR (CD_3OD, 500 MHz)



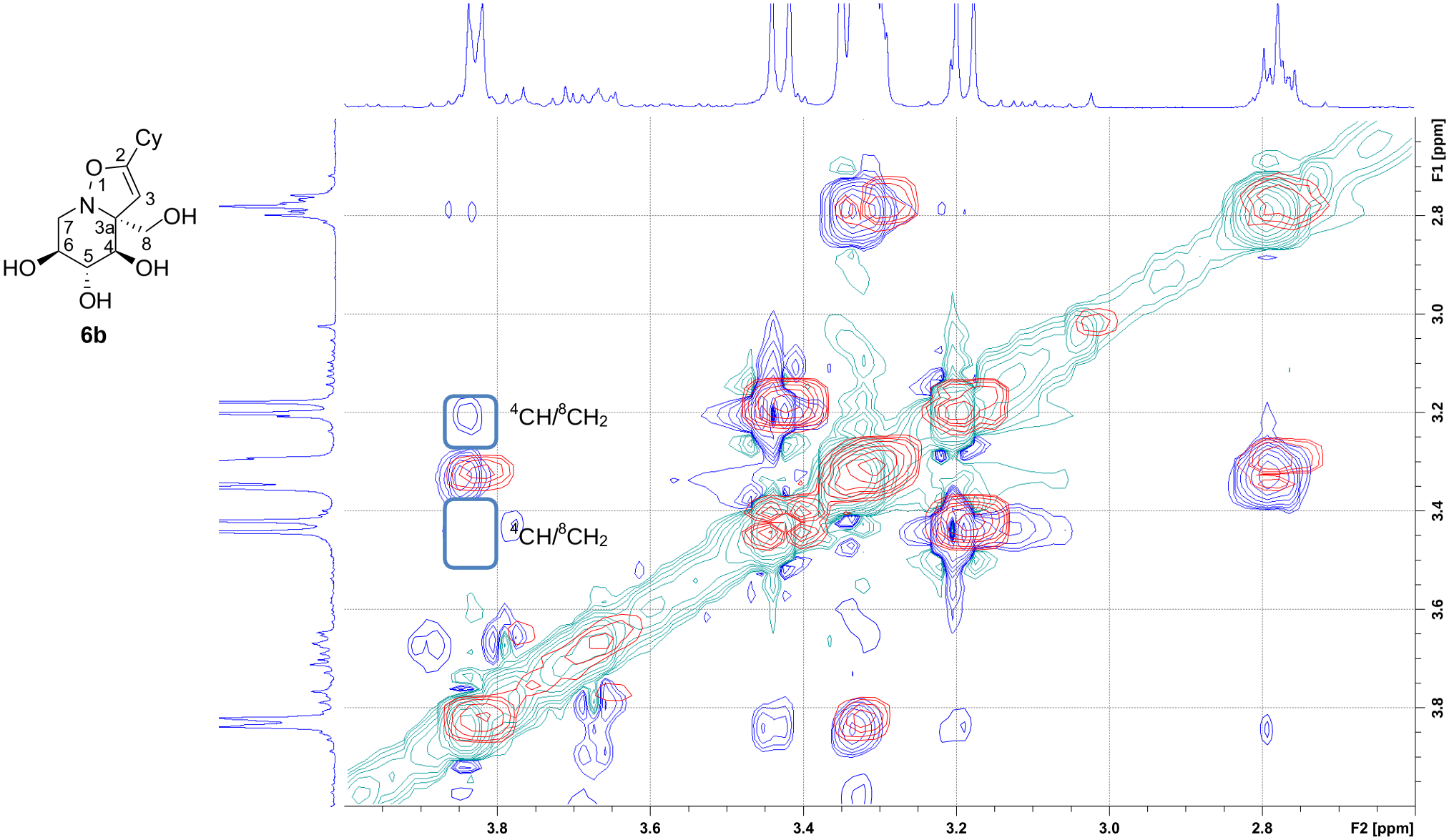
6b

^{13}C NMR (CD_3OD, 125 MHz)

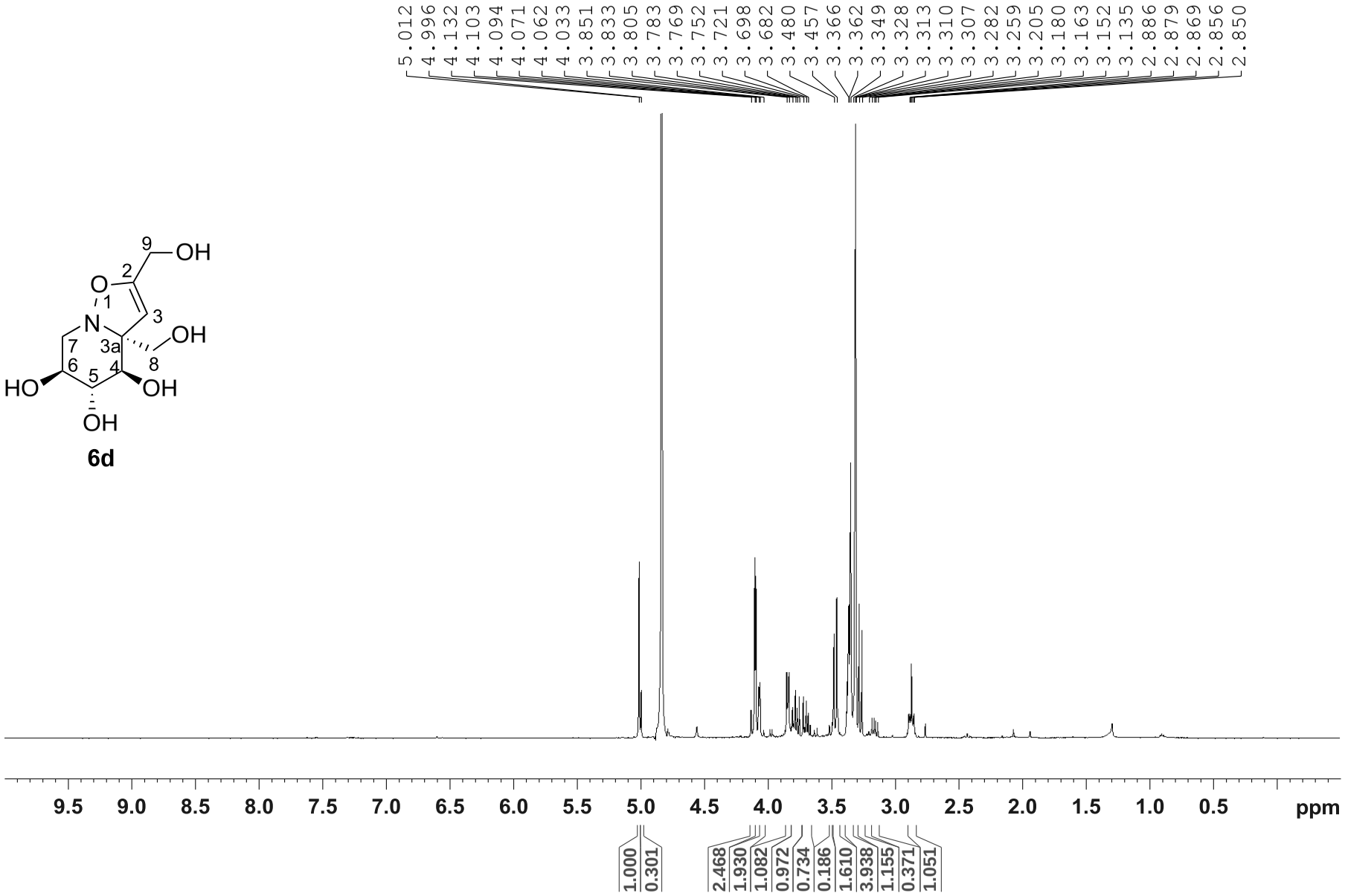


6b

NOESY (blue), COSY (red) correlations (CD_3OD, 500 MHz)

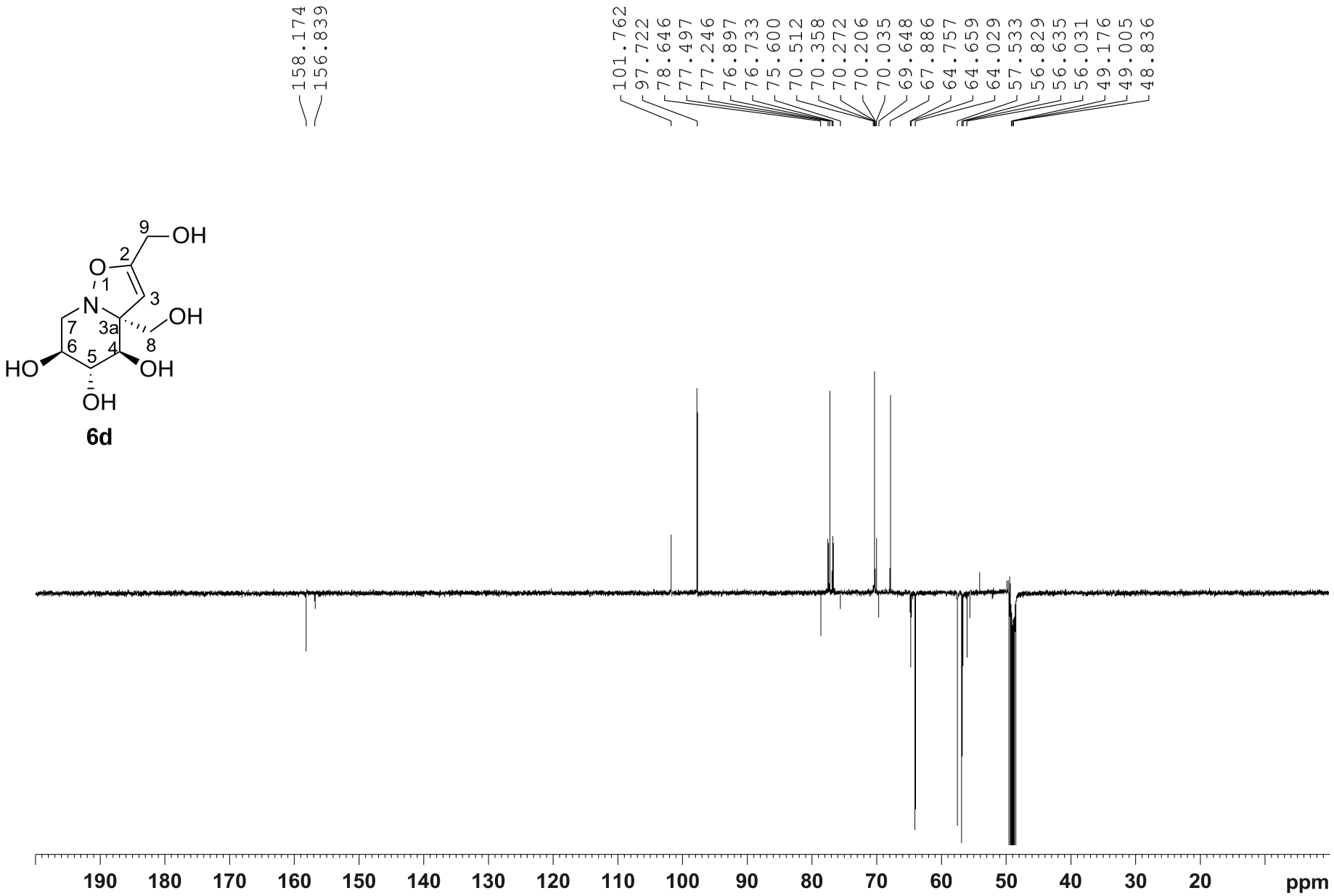


^{1}H NMR (CD_3OD, 500 MHz)



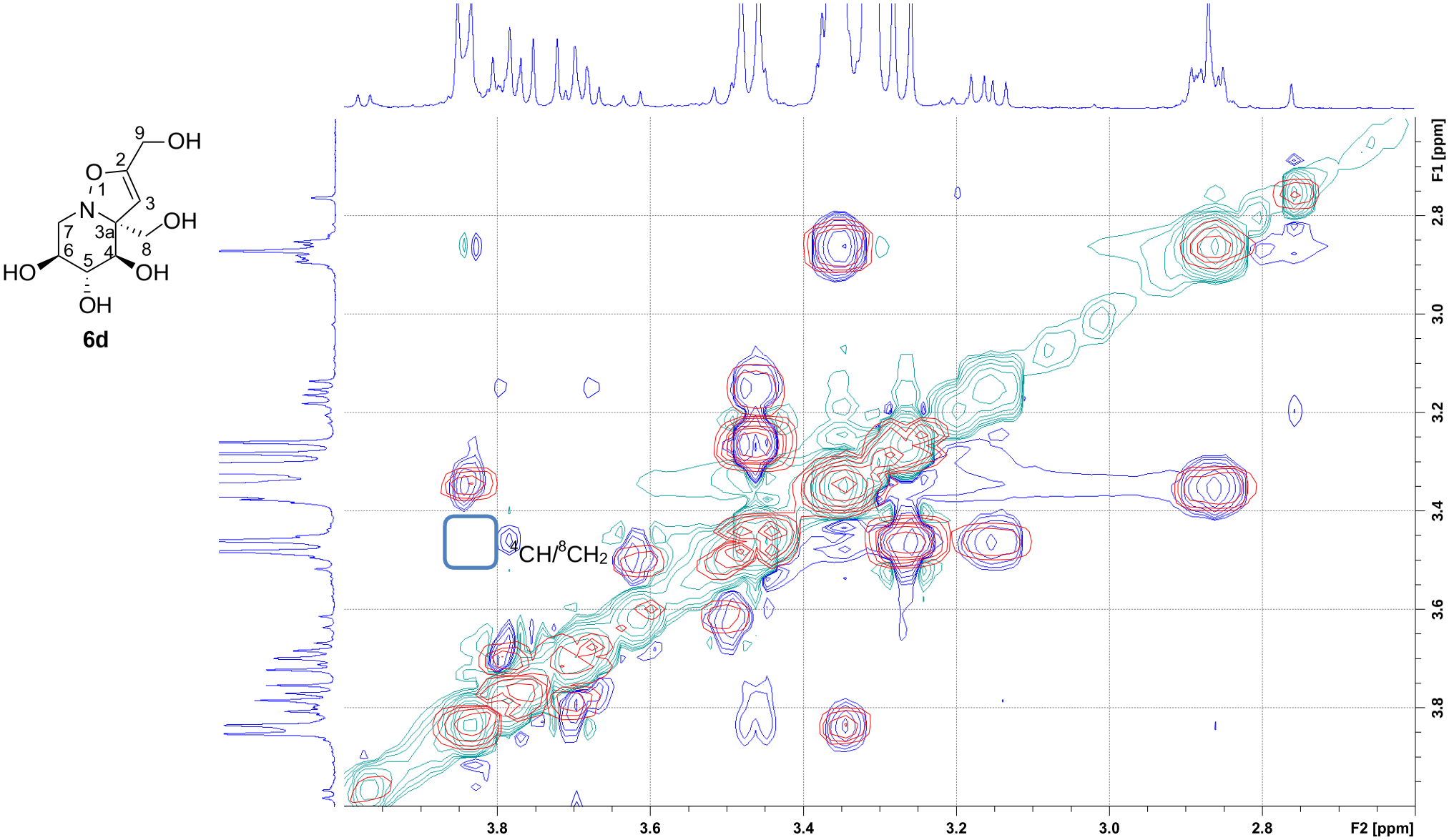
6d

^{13}C NMR (CD_3OD, 125 MHz)



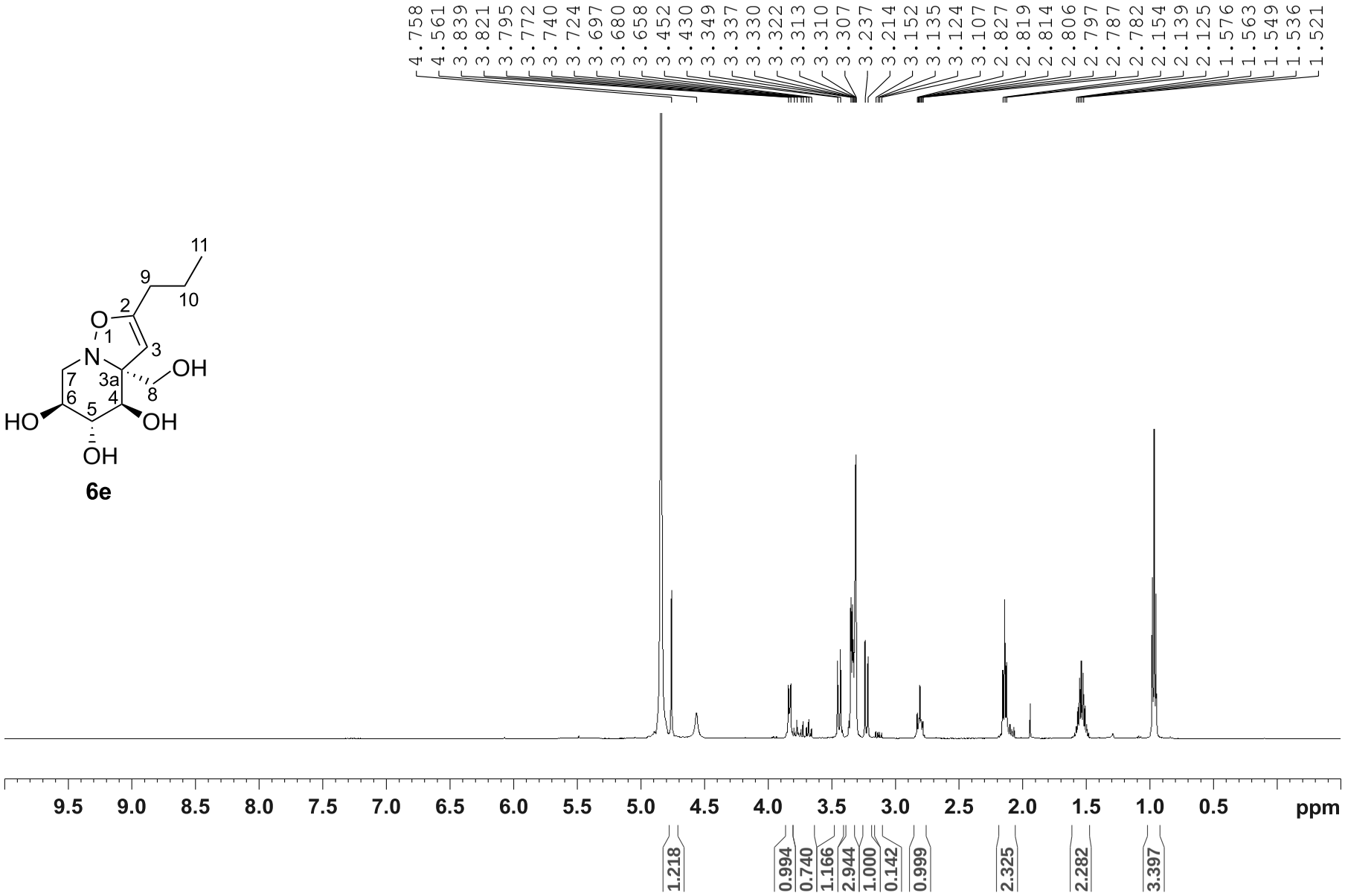
6d

NOESY (blue), COSY (red) correlations (CD_3OD, 500 MHz)



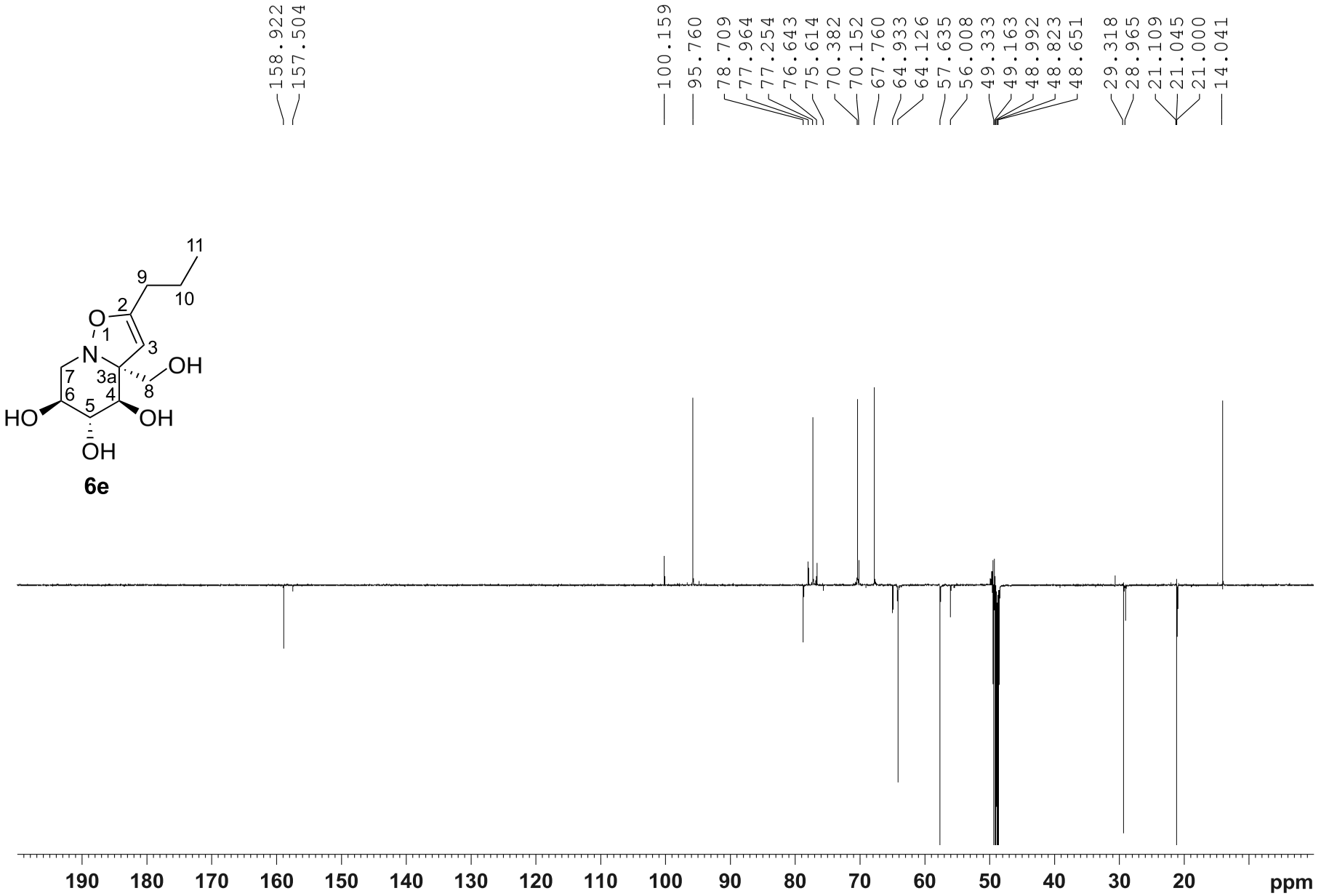
6d

^{1}H NMR (CD_3OD, 500 MHz)

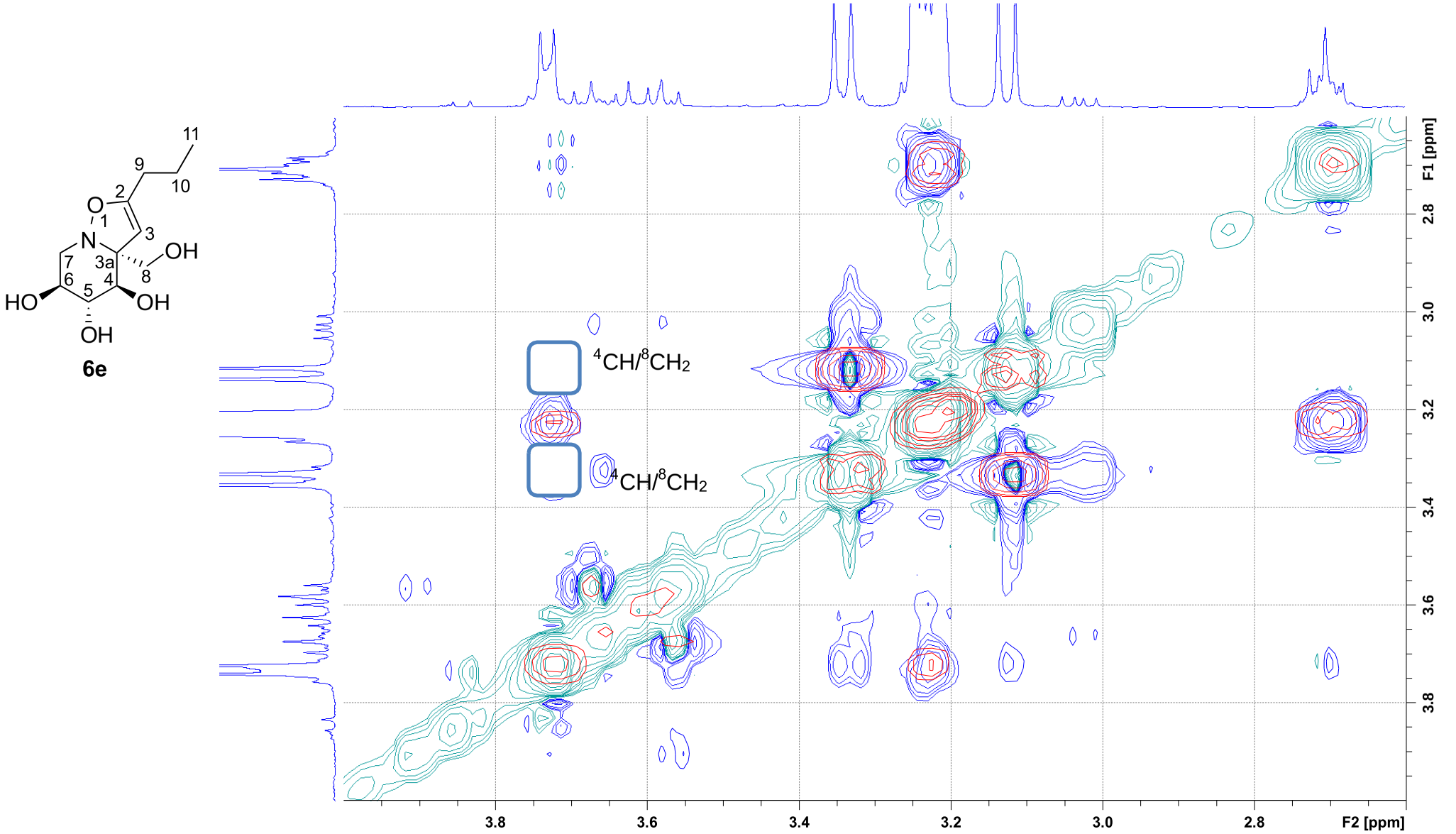


6e

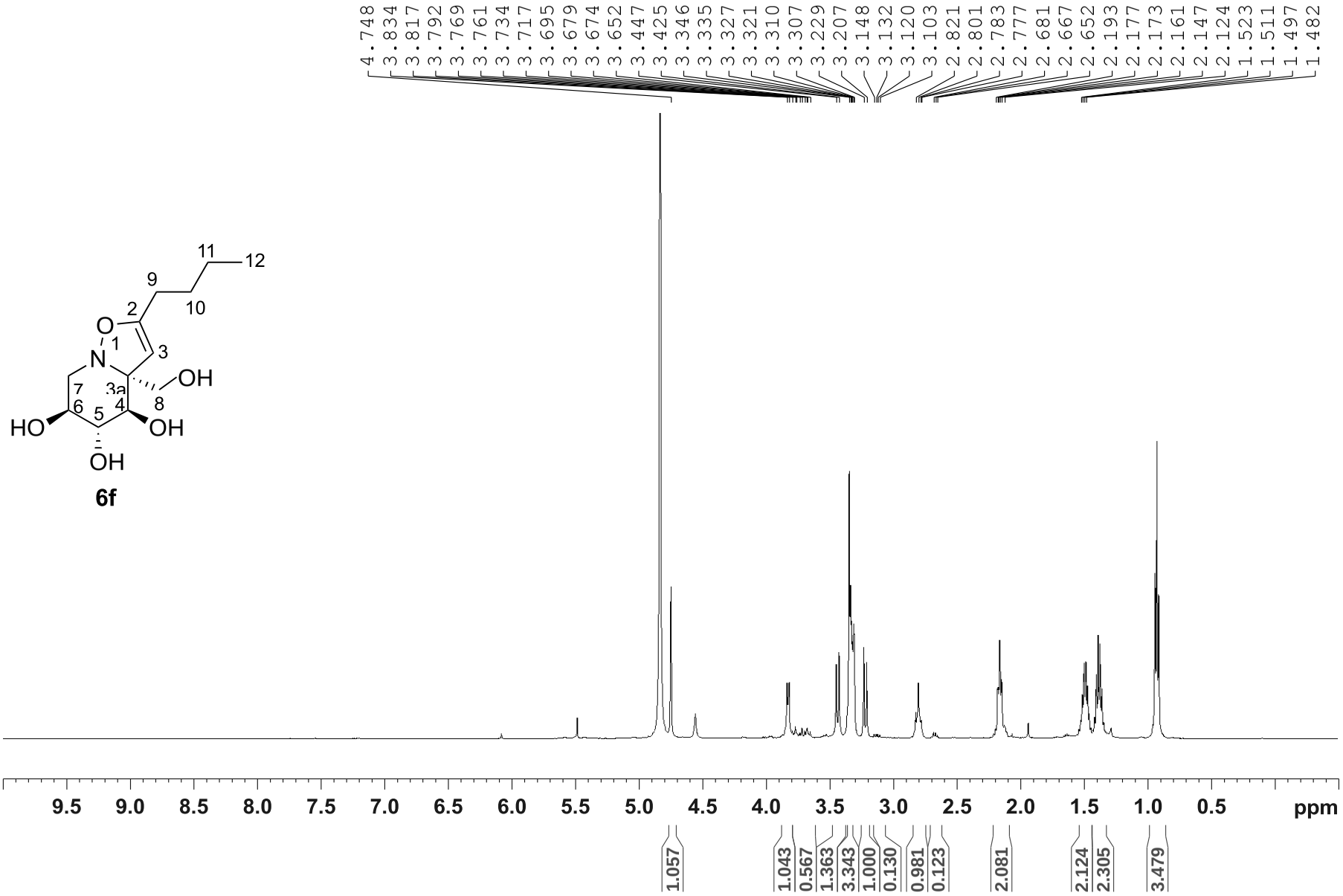
^{13}C NMR (CD_3OD, 125 MHz)



NOESY (blue), COSY (red) correlations (CD_3OD, 500 MHz)

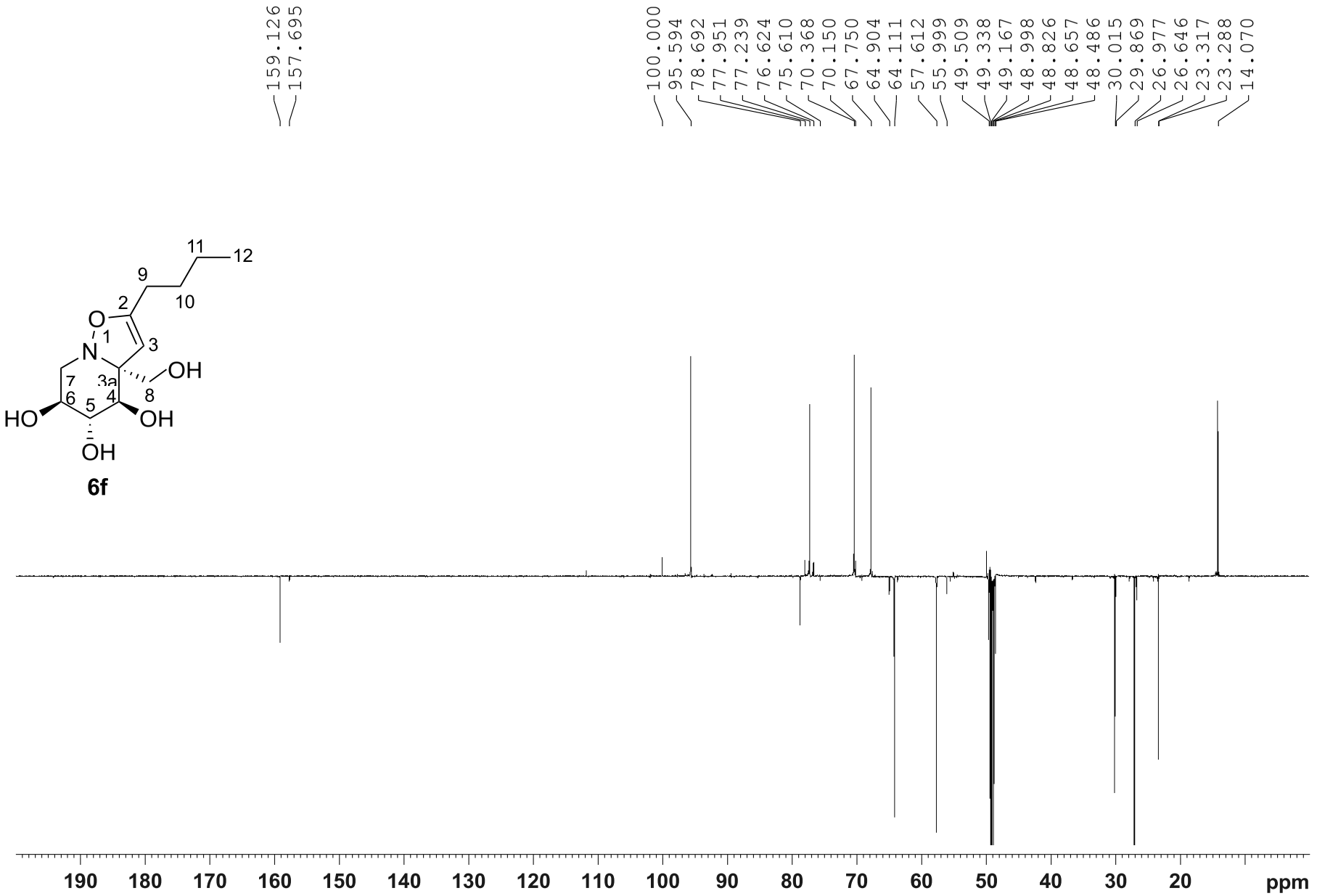


^{1}H NMR (CD_3OD, 500 MHz)



6f

^{13}C NMR (CD_3OD, 125 MHz)



NOESY (blue), COSY (red) correlations (CD_3OD, 500 MHz)