Supporting Information for

Cyclometalated Ruthenium Complexes with Carboxylated Ligands from a Combined Experimental/Computational Perspective

Contents

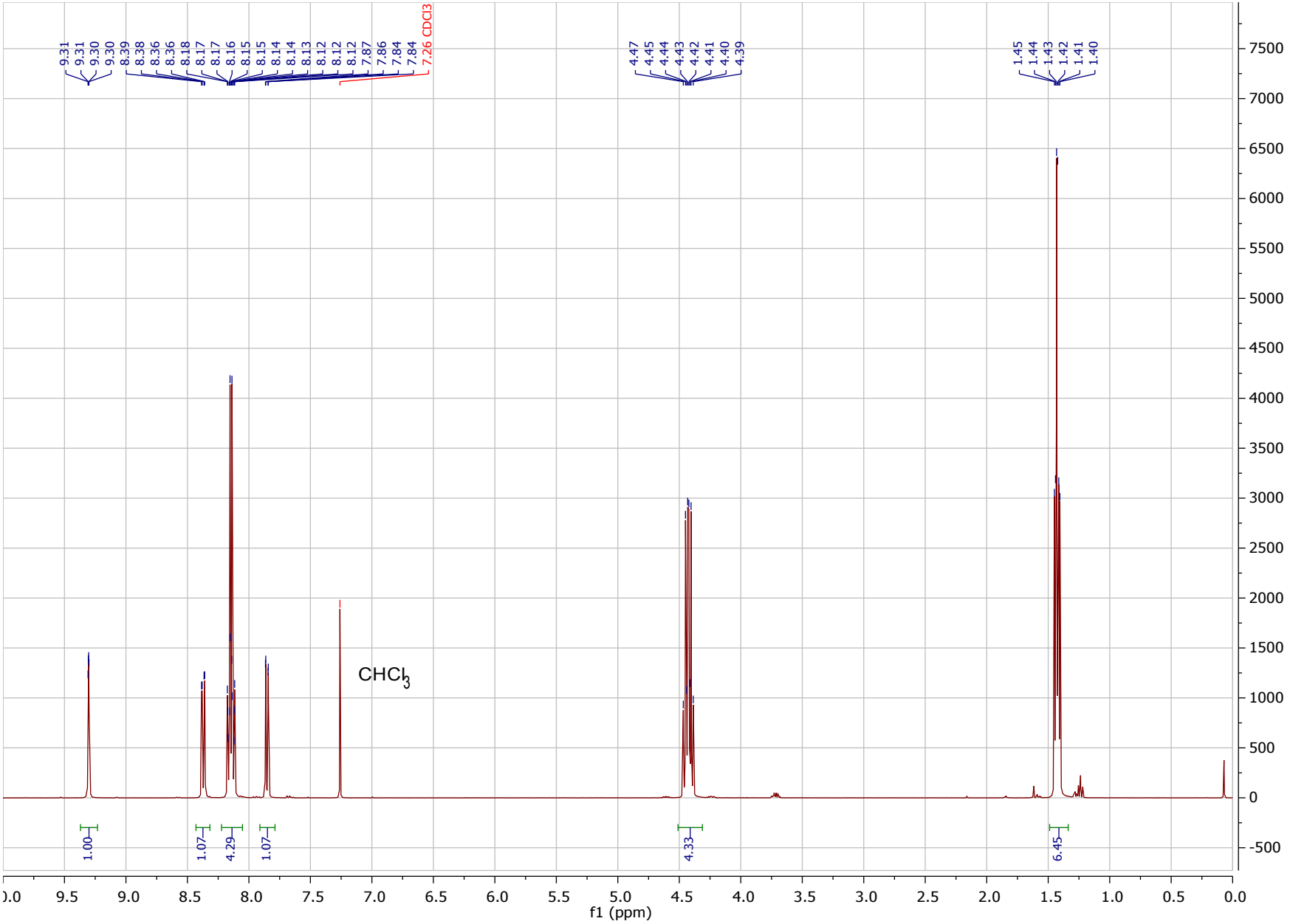

Figure S1. ^{1}H NMR spectrum of Ethyl 6-(4-(ethoxycarbonyl)phenyl)pyridine-3-carboxylate. $CDCl_3$, 400 MHz.

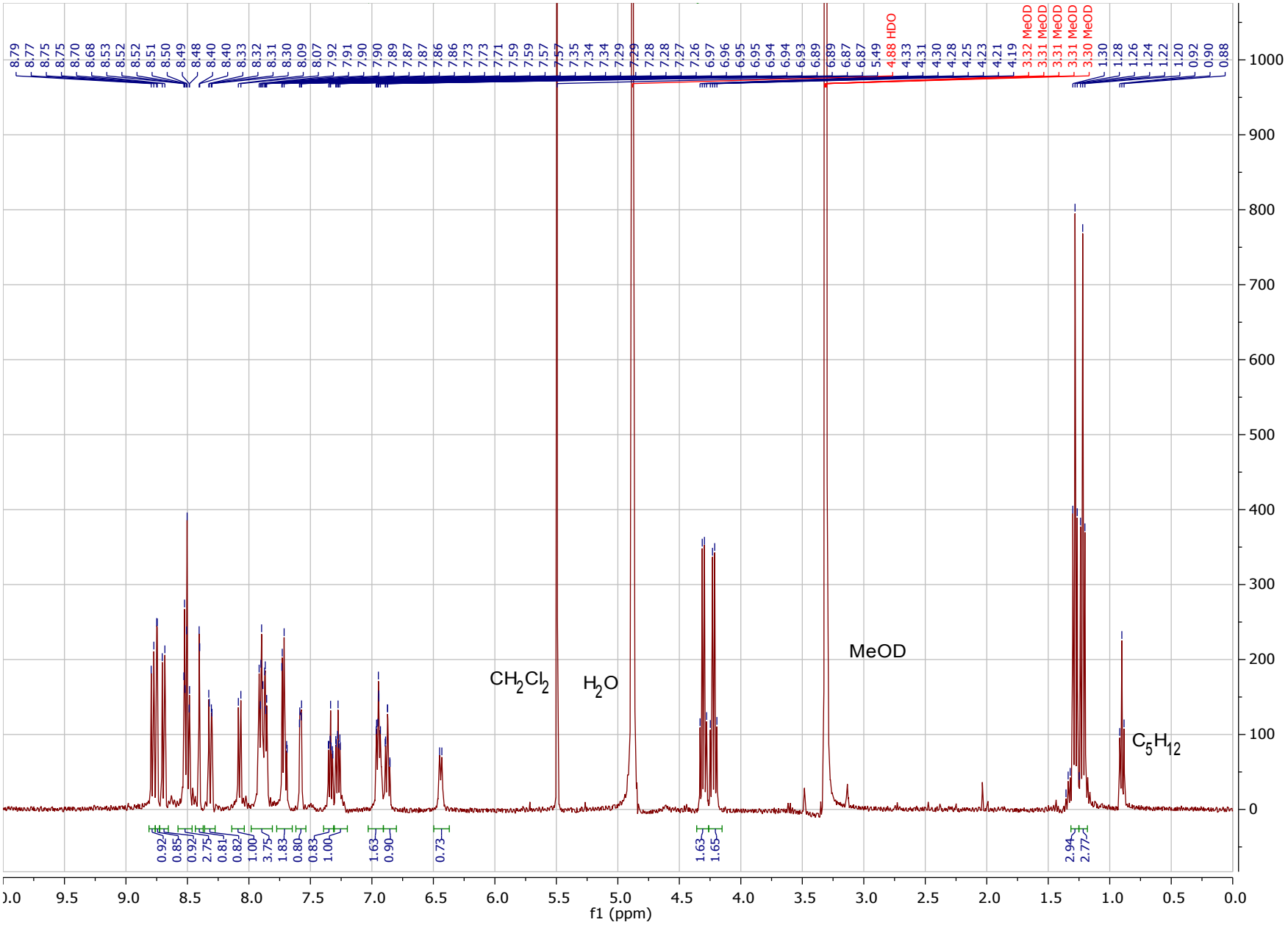

Figure S2. ^{1}H NMR spectrum of compound 2-Et. CD_3OD, 400 MHz.

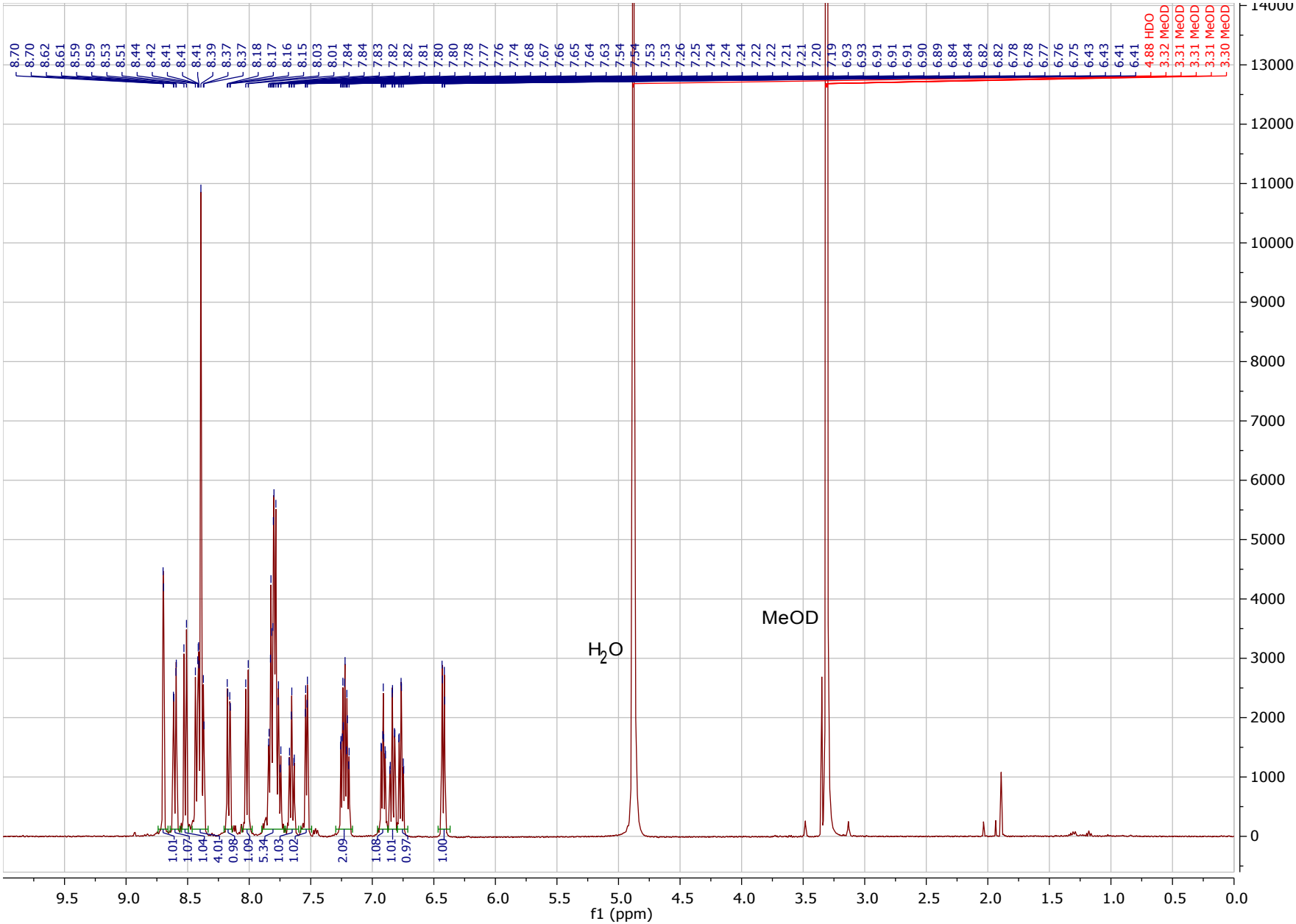

Figure S3. ^{1}H NMR spectrum of compound 2-Na. CD_3OD, 400 MHz.

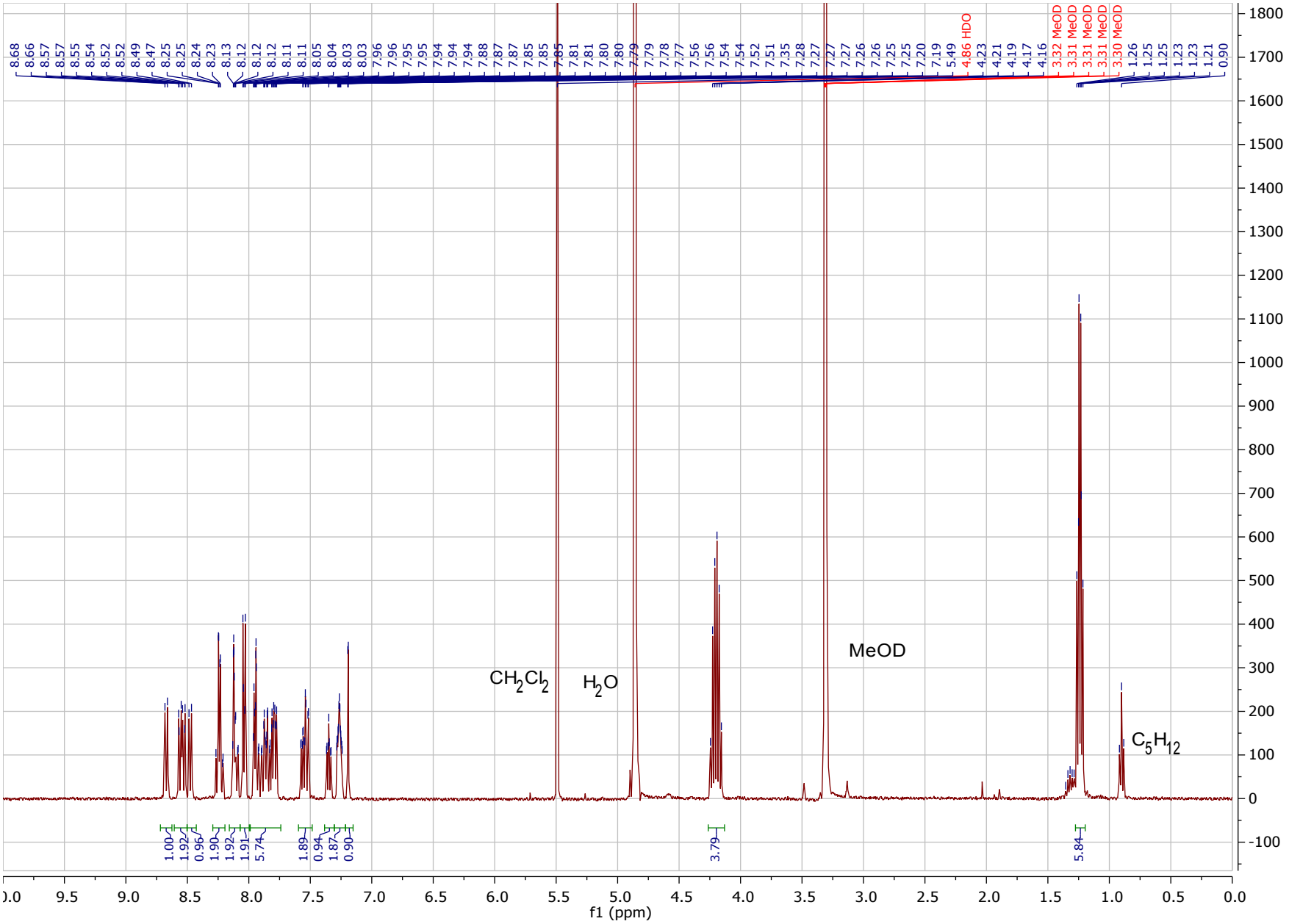

Figure S4. ^{1}H NMR spectrum of compound 3-Et. CD_3OD, 400 MHz.

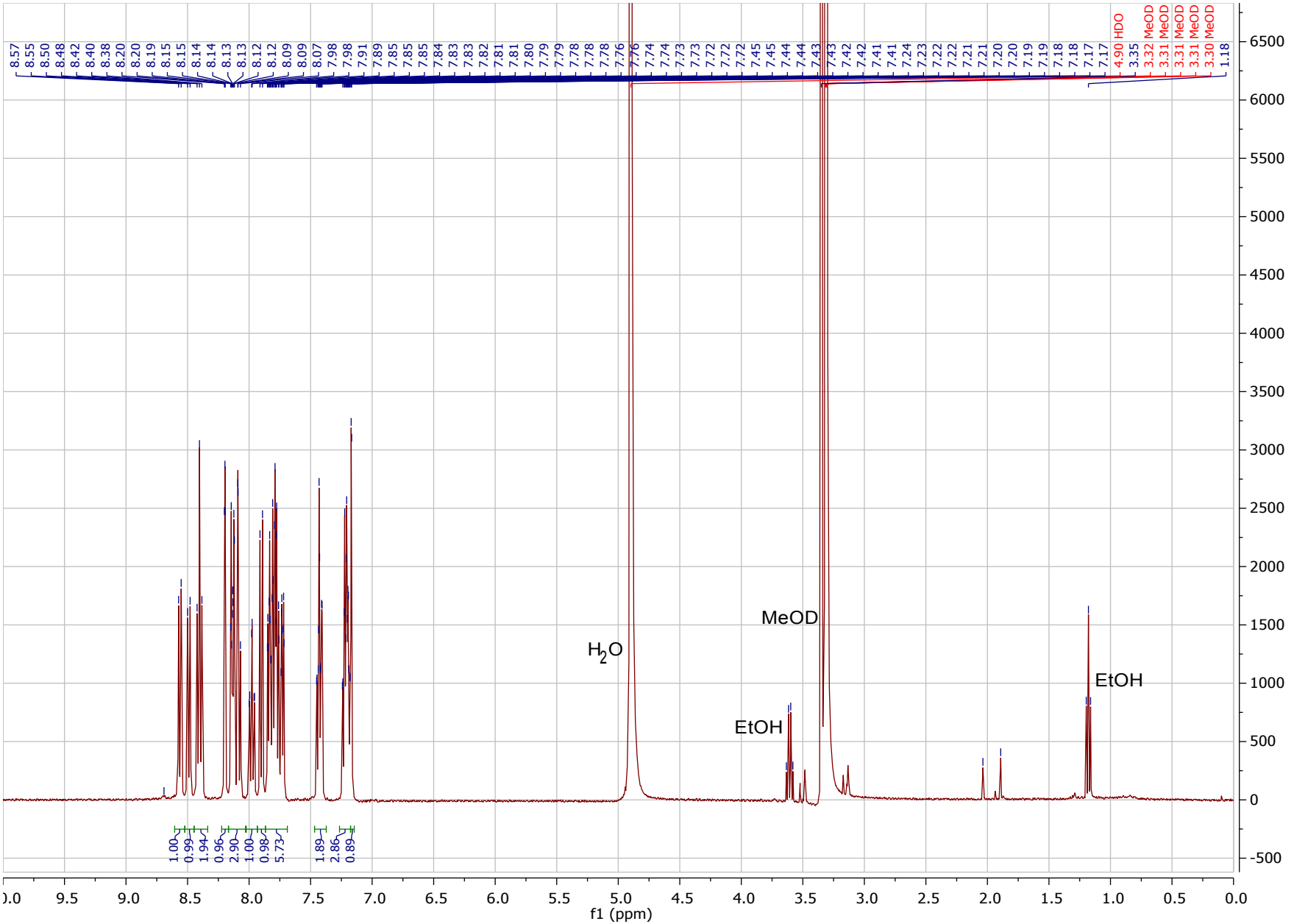

Figure S5. ^{1}H NMR spectrum of compound 3-Na. CD_3OD, 400 MHz.

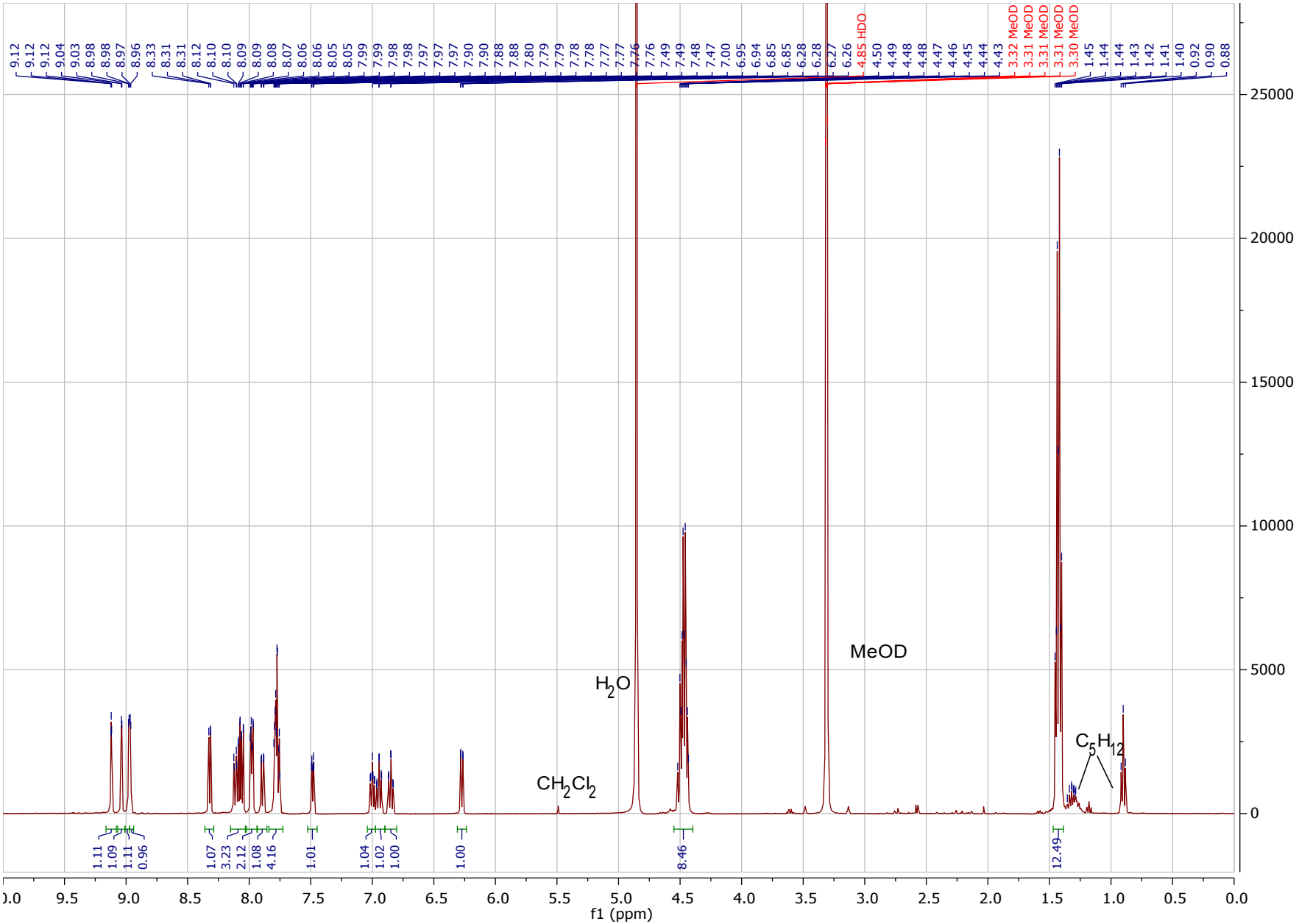

Figure S6. ^{1}H NMR spectrum of compound 4-Et. CD_3OD, 400 MHz.

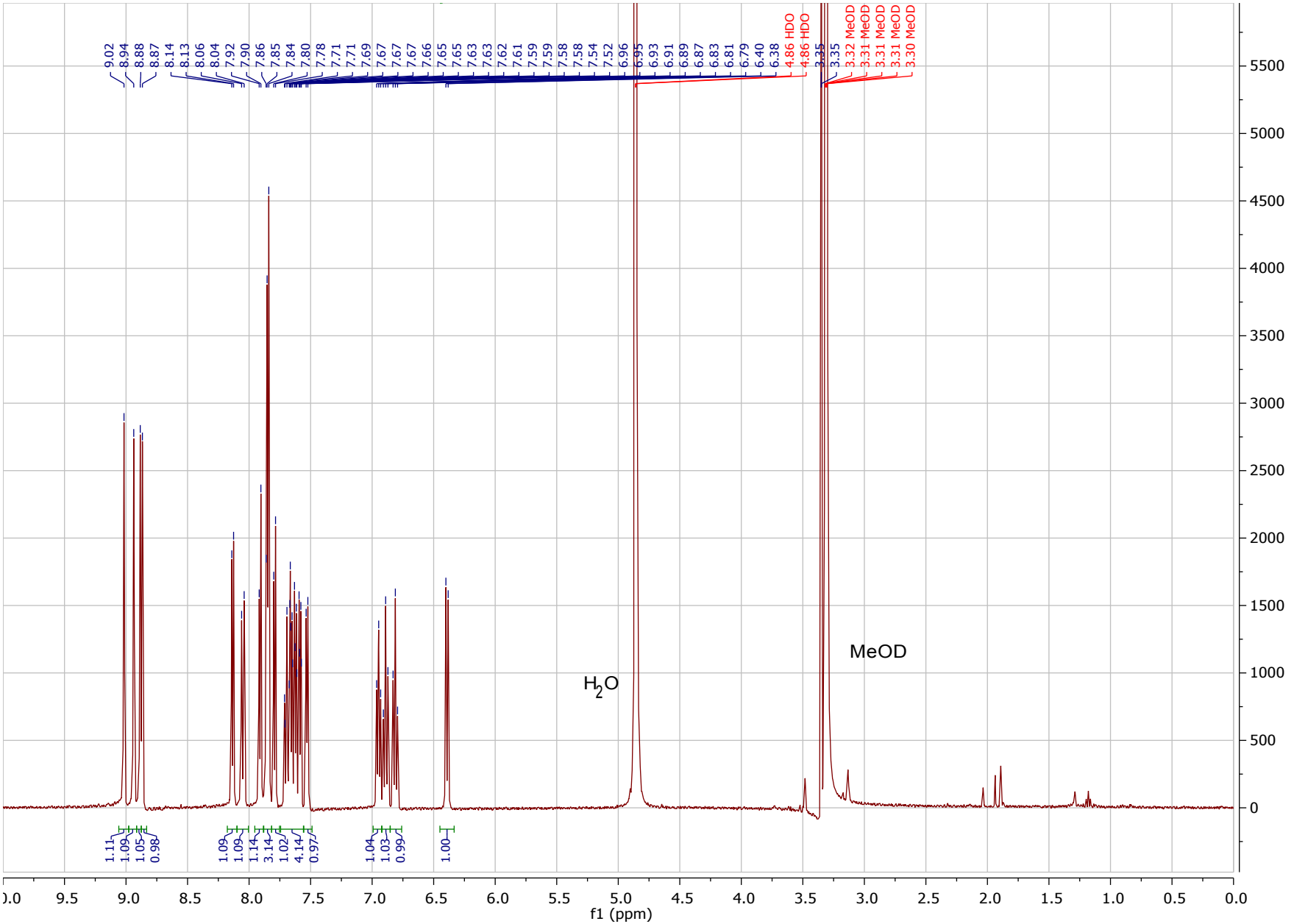

Figure S7. ^{1}H NMR spectrum of compound 4-Na. CD_3OD, 400 MHz.

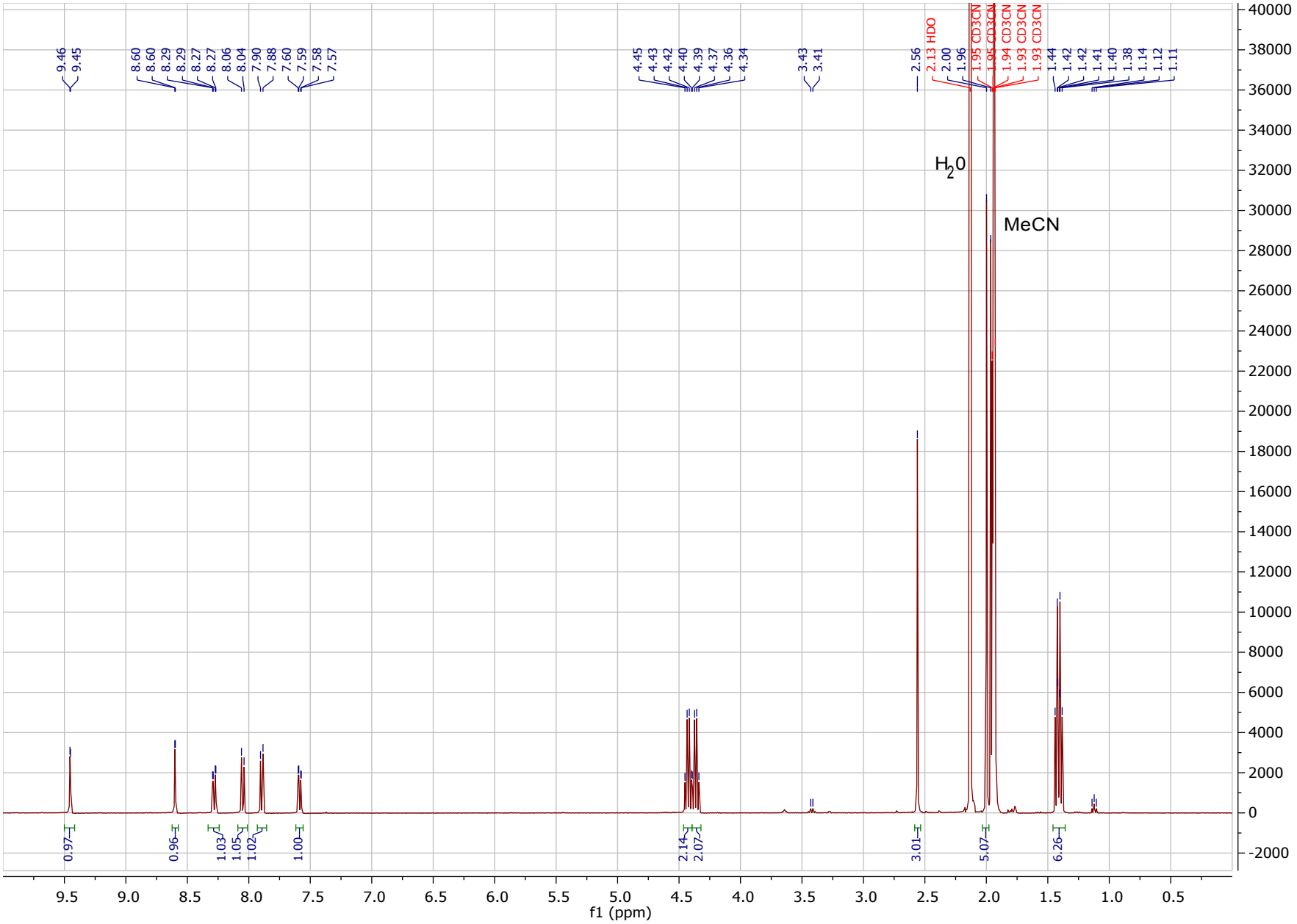

Figure S8. ^{1}H NMR spectrum of compound 5-Et. CD_3CN, 400 MHz.

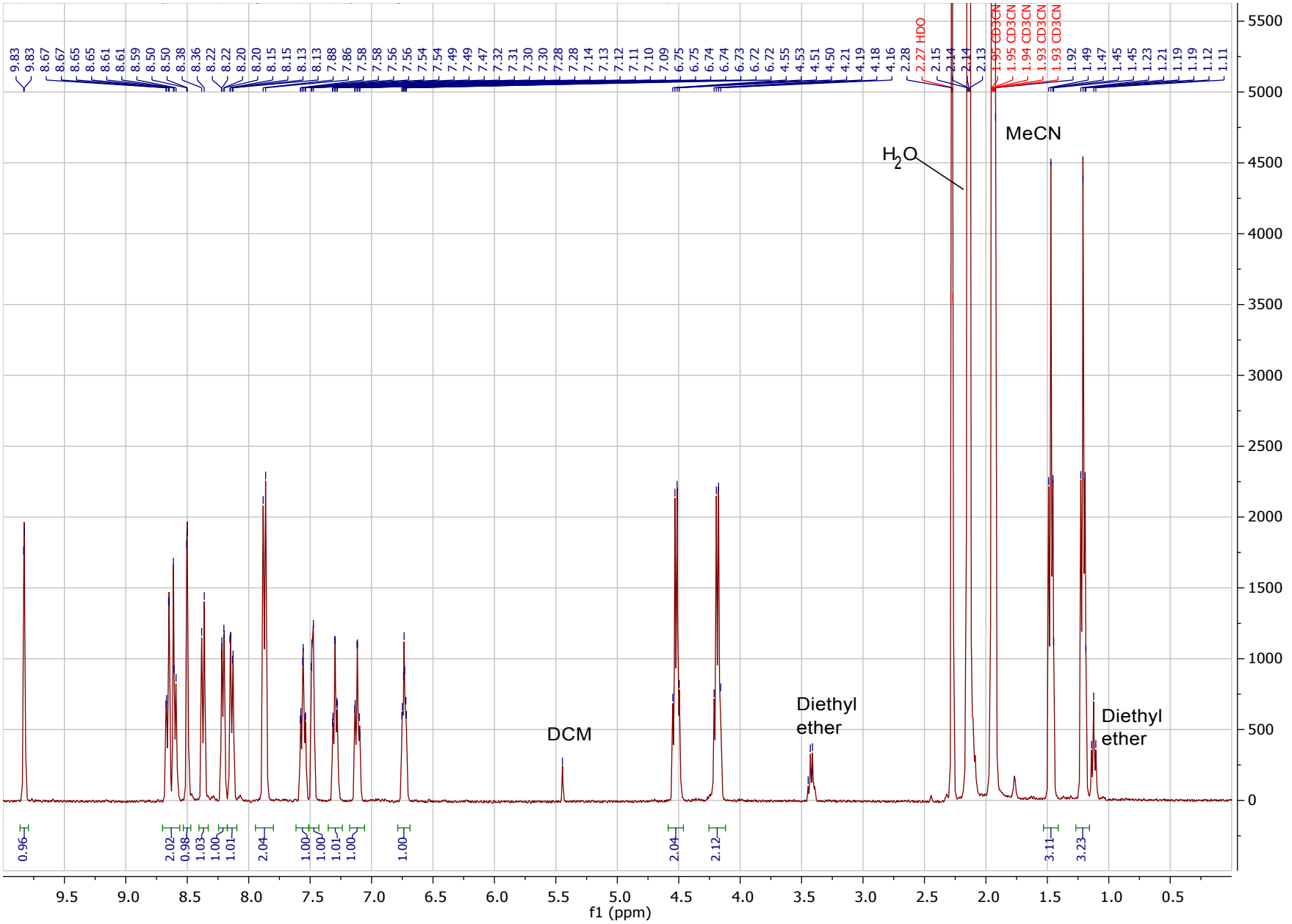

Figure S9. ^{1}H NMR spectrum of compound 6-Et. CD_3CN, 400 MHz.

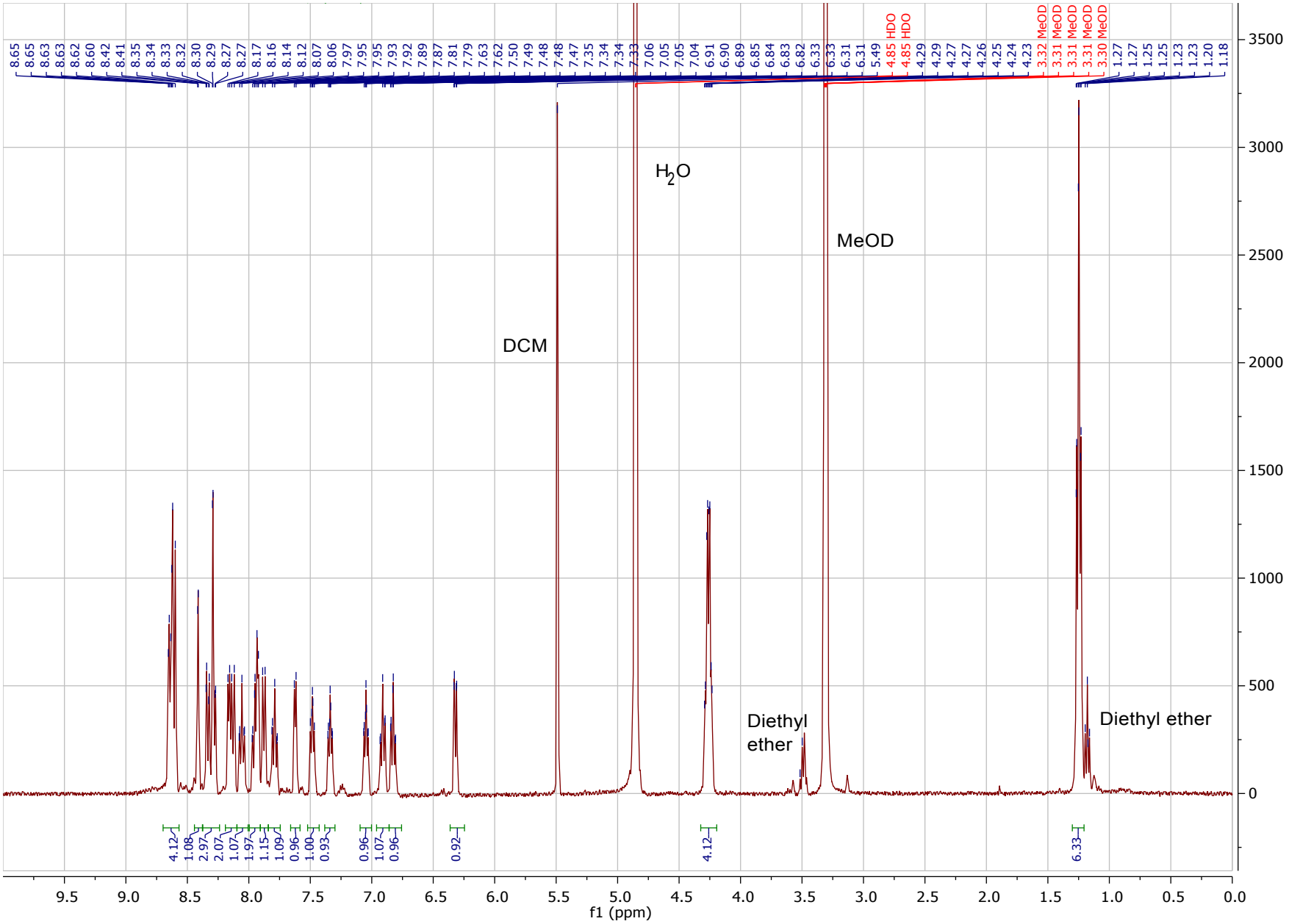

Figure S10. ^{1}H NMR spectrum of compound 7-Et. CD_3OD, 400 MHz.

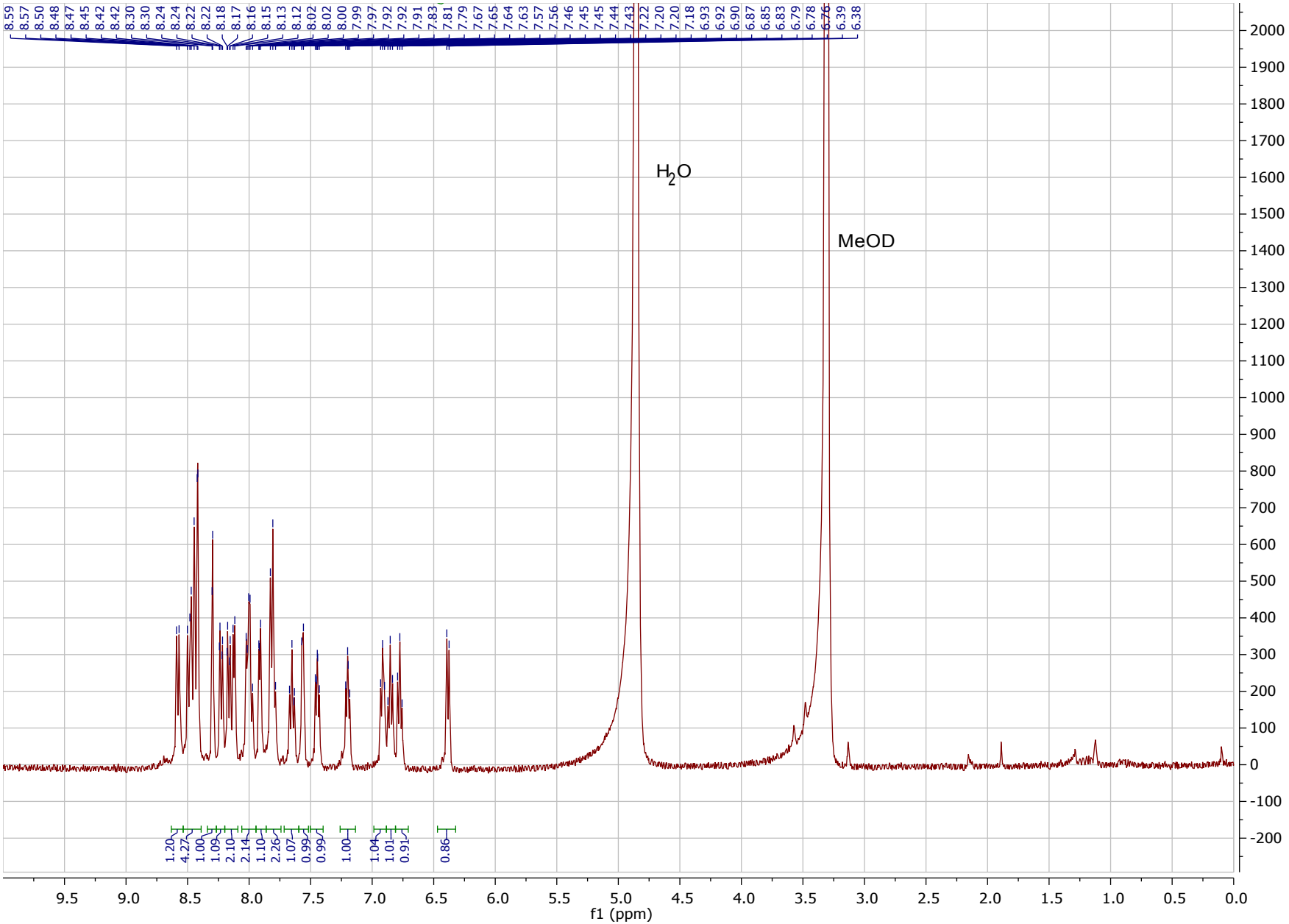

Figure S11. ^{1}H NMR spectrum of compound 7-Na. CD_3OD, 400 MHz.

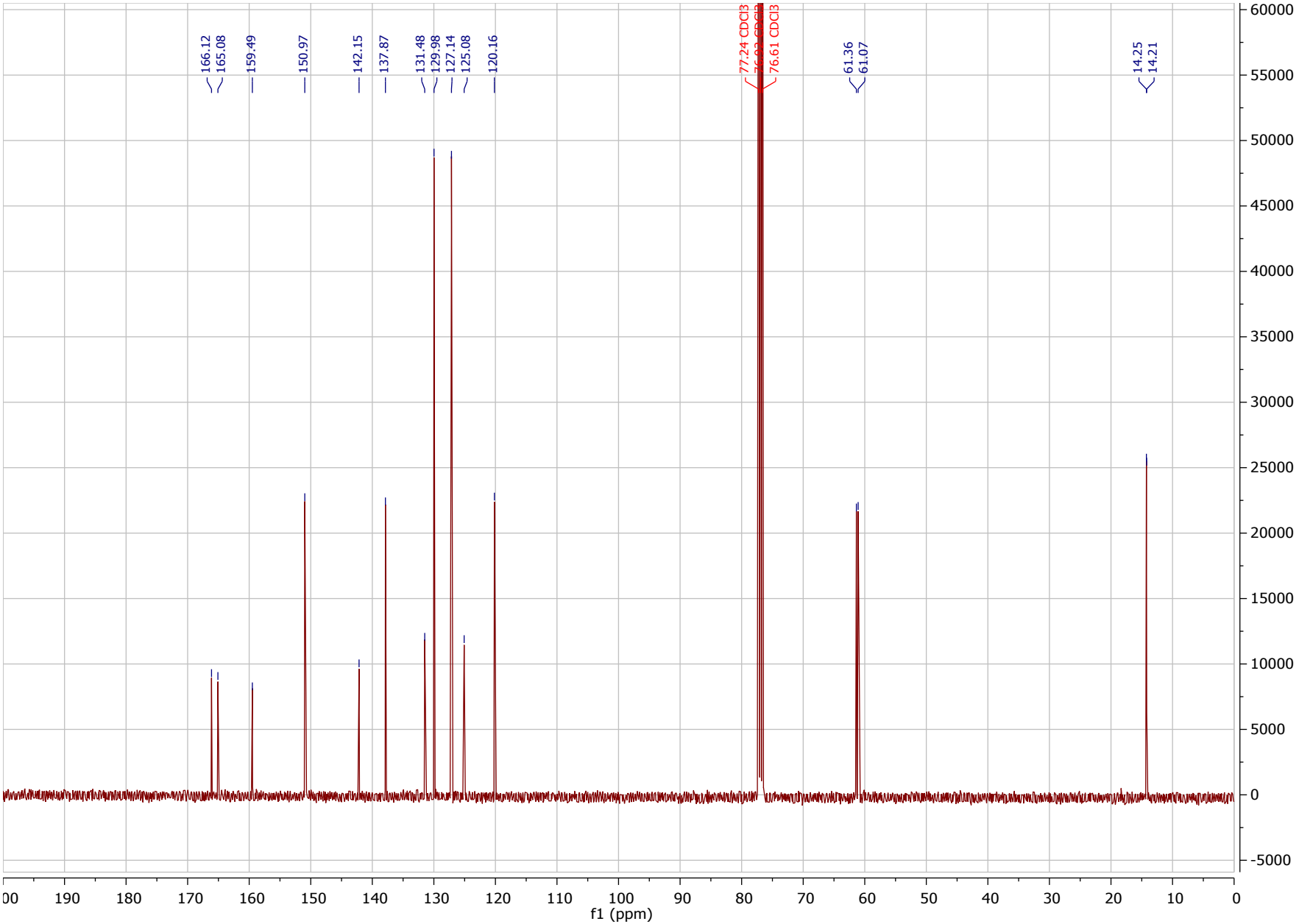

Figure S12. ^{13}**C NMR spectrum of ethyl 6-(4-(ethoxycarbonyl)phenyl)pyridine-3-carboxylate.** $CDCl_3$**, 100 MHz.**

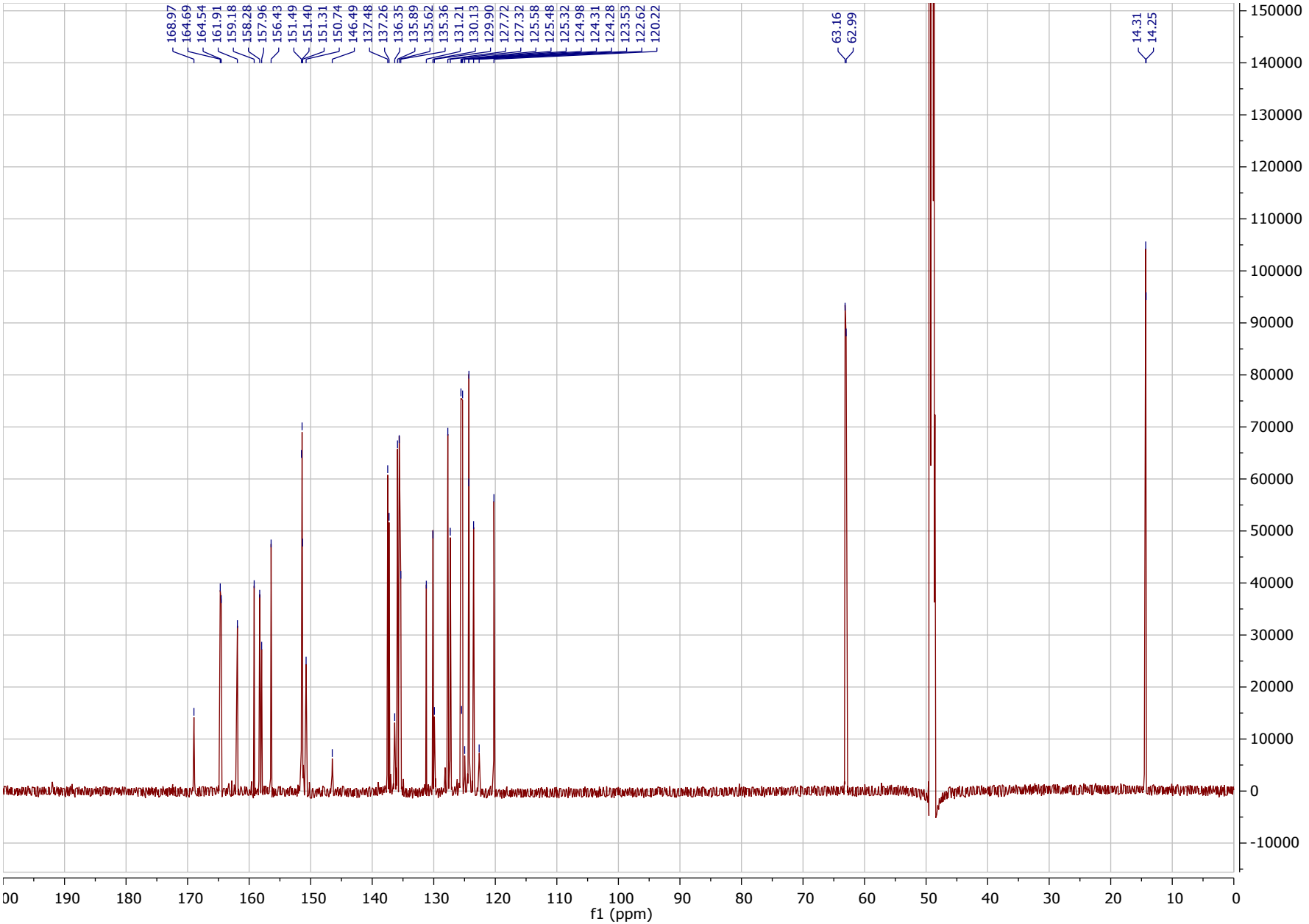

Figure S13. ^{13}C NMR spectrum of compound 2-Et. CD_3OD, 151 MHz.

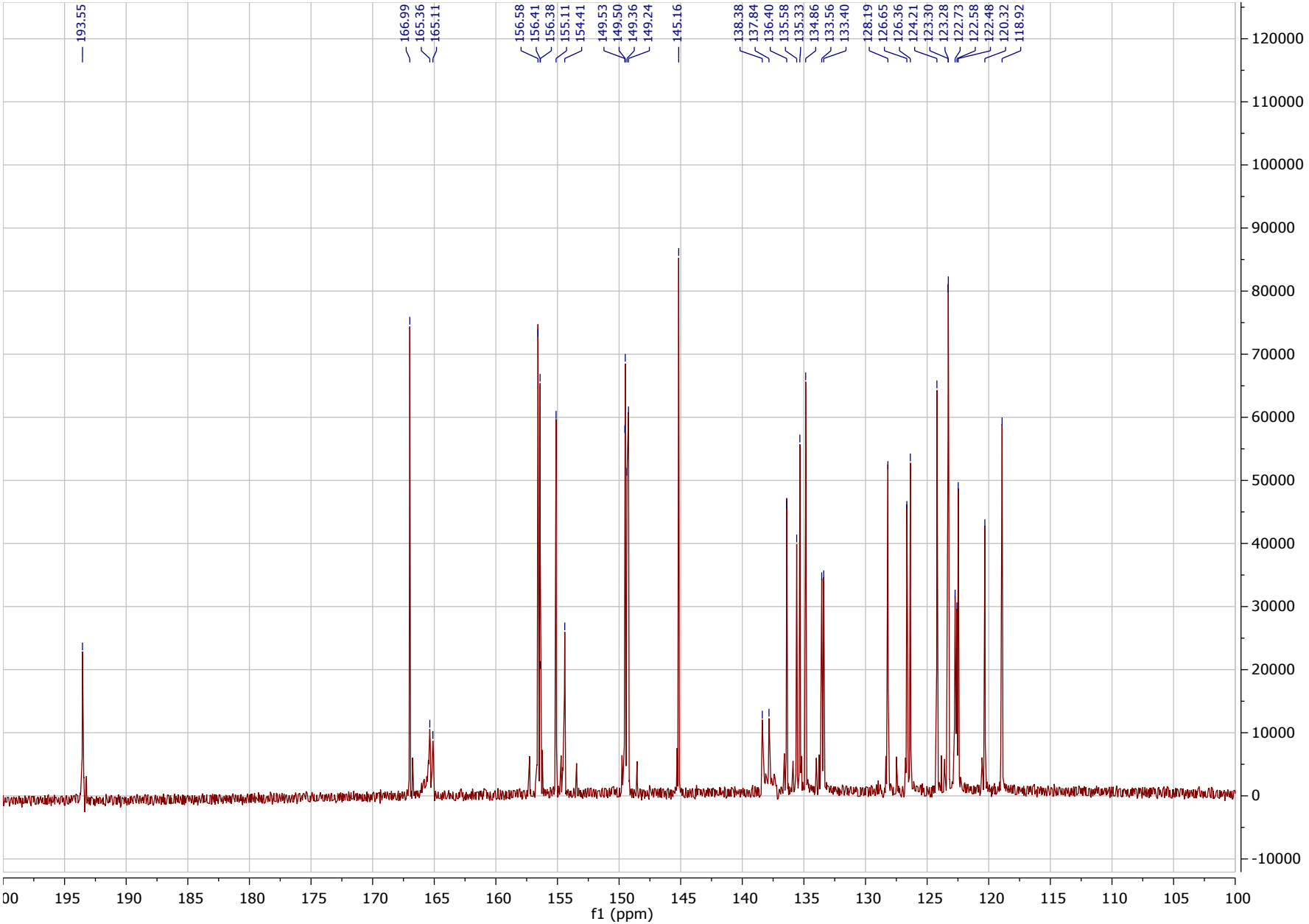

Figure S14. ^{13}C NMR spectrum of compound 2-Na. DMSO, 151 MHz.

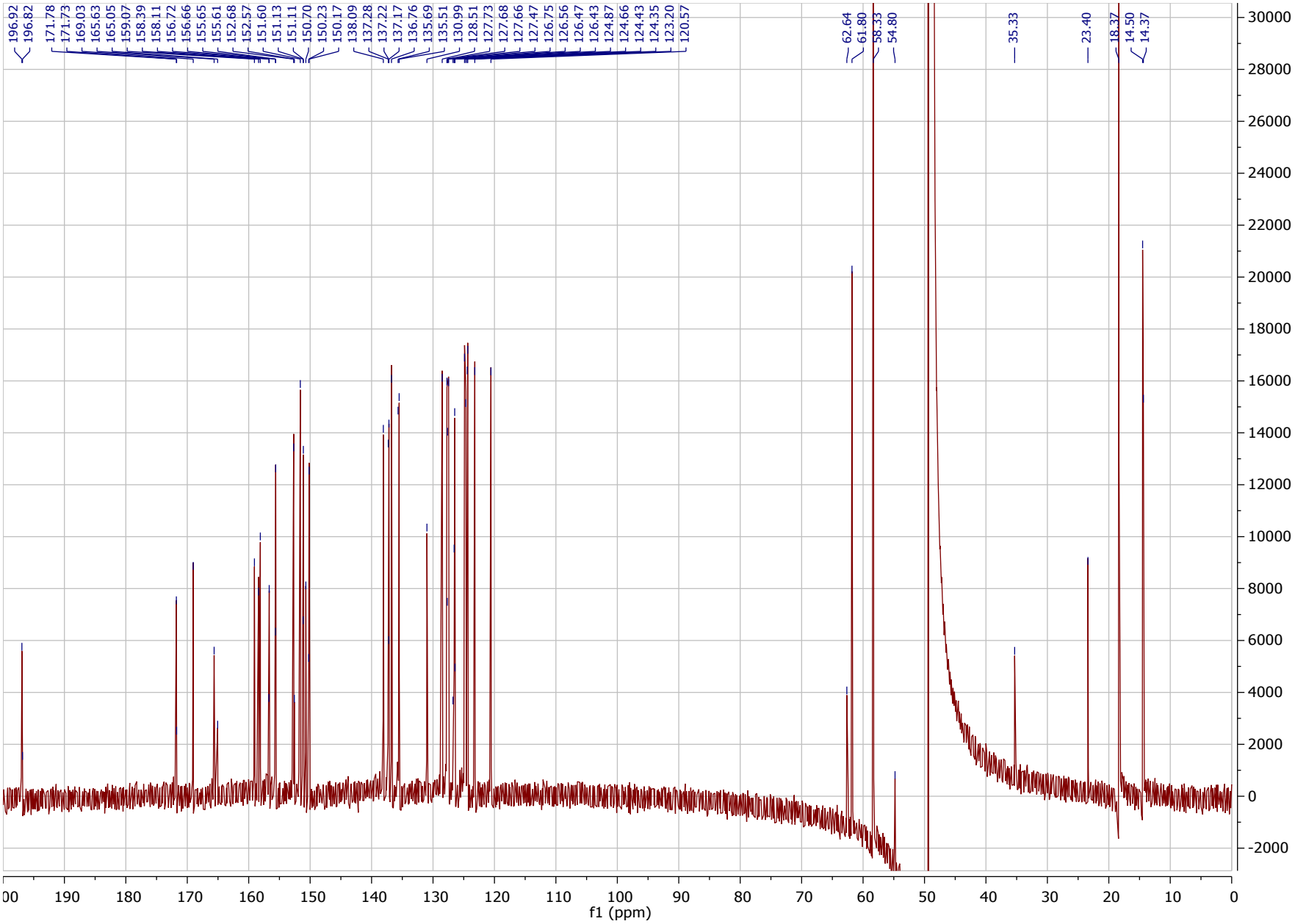

Figure S15. ^{13}C NMR spectrum of compound 3-Et. CD_3OD, 151 MHz.

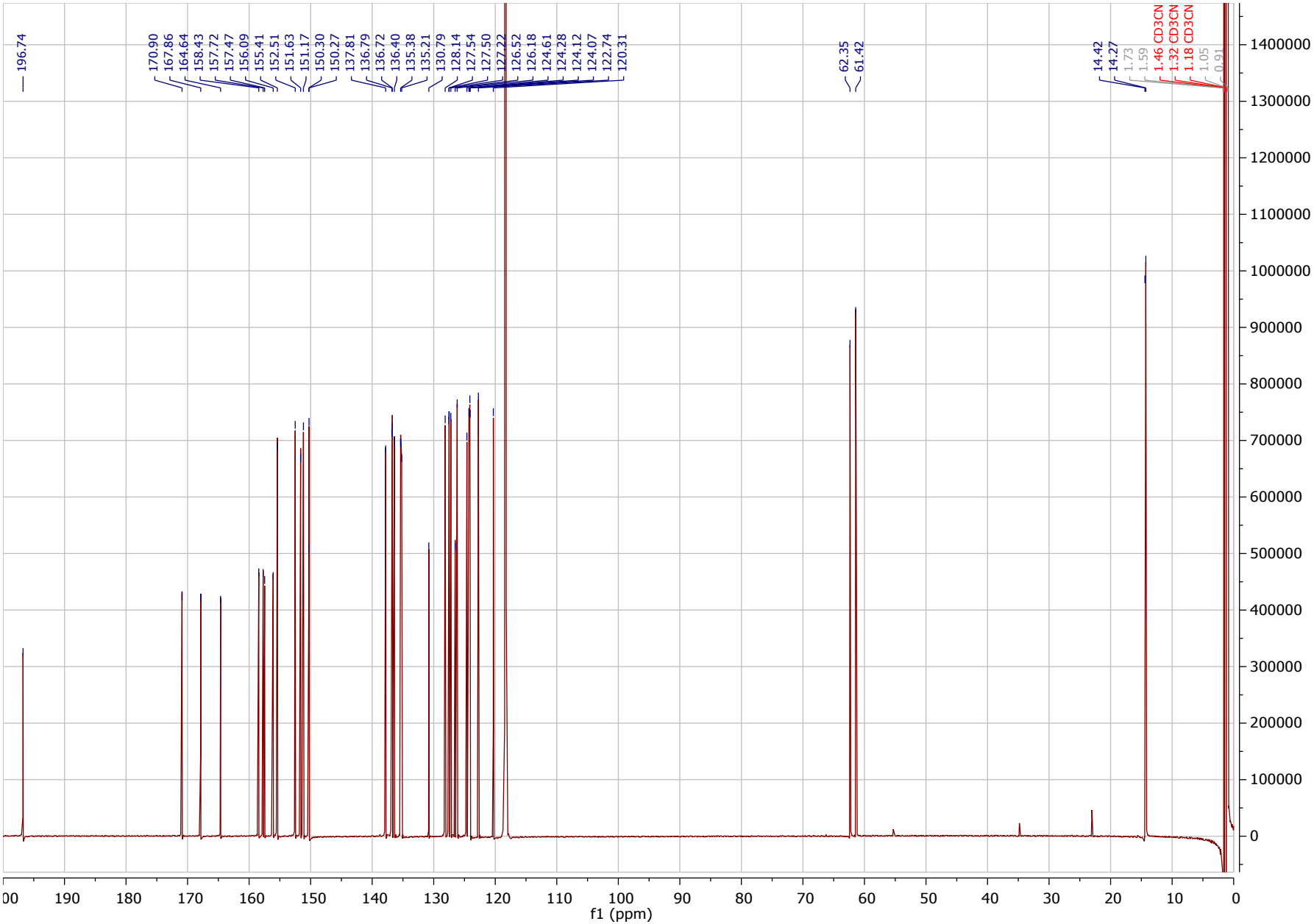

Figure S16. ^{13}C NMR spectrum of compound 3-Et. CD_3CN, 151 MHz.

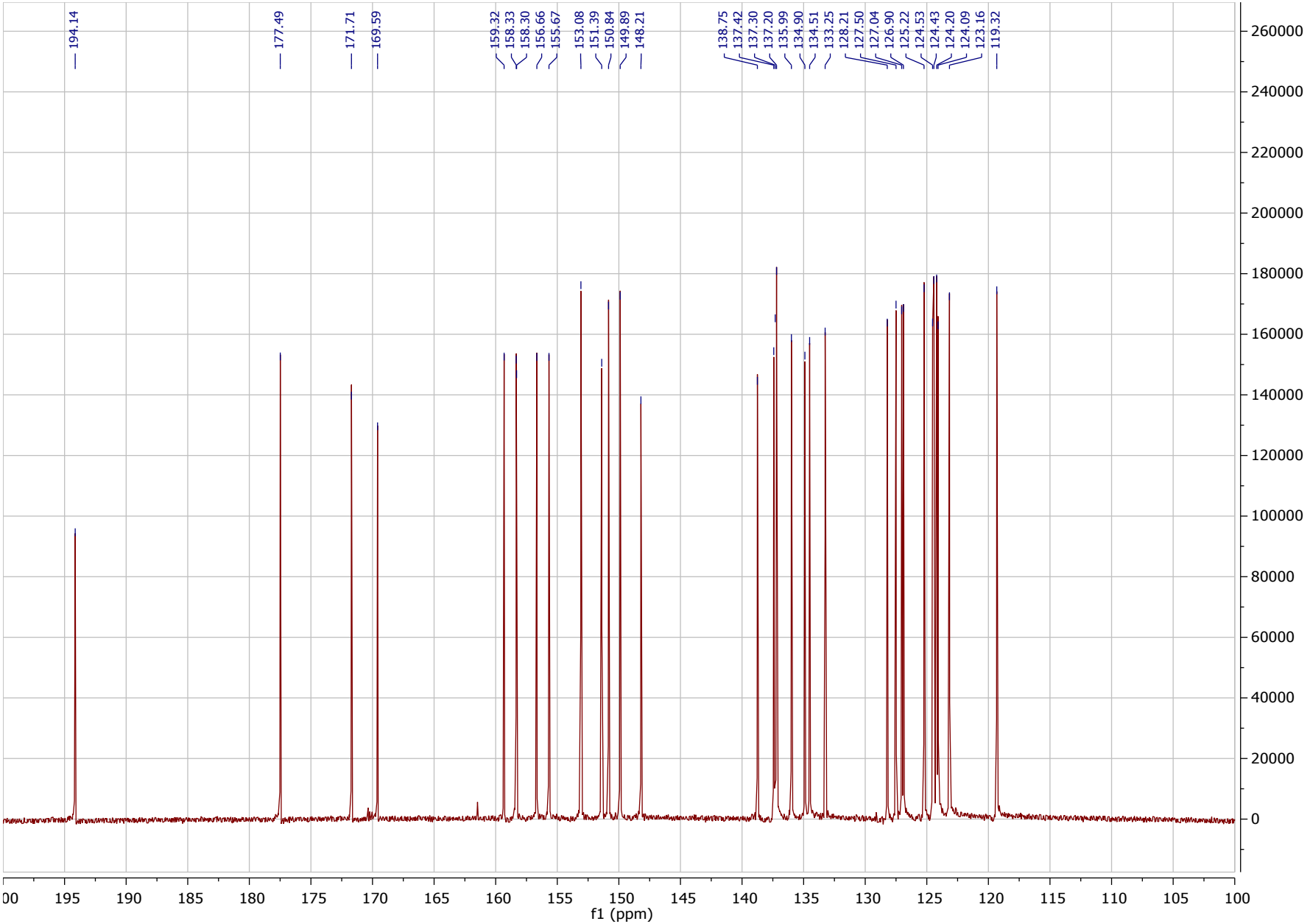

Figure S17. ^{13}C NMR spectrum of compound 3-Na. CD_3OD, 151 MHz.

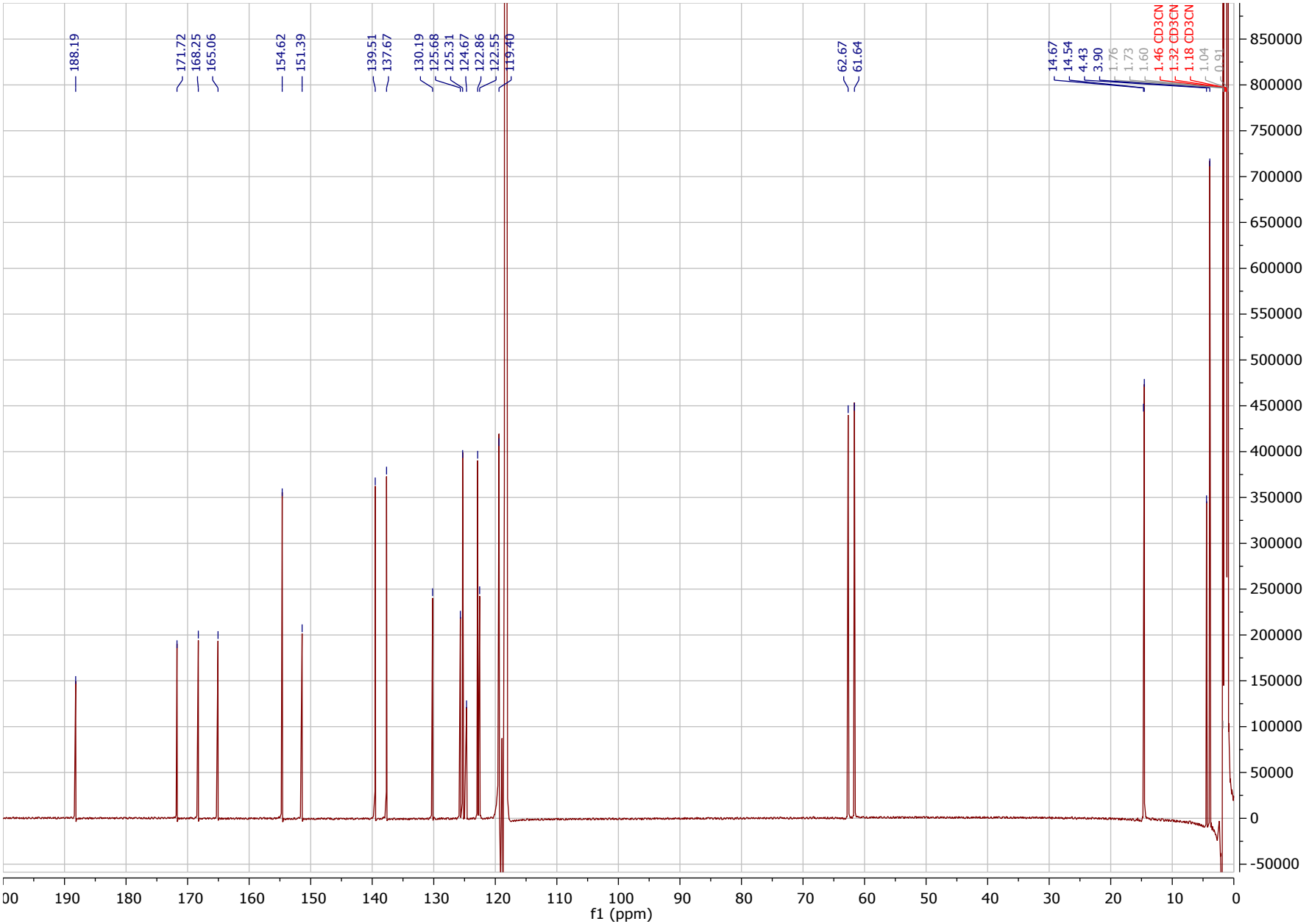

Figure S18. ^{13}C NMR spectrum of compound 5-Et. CD_3CN, 151 MHz.

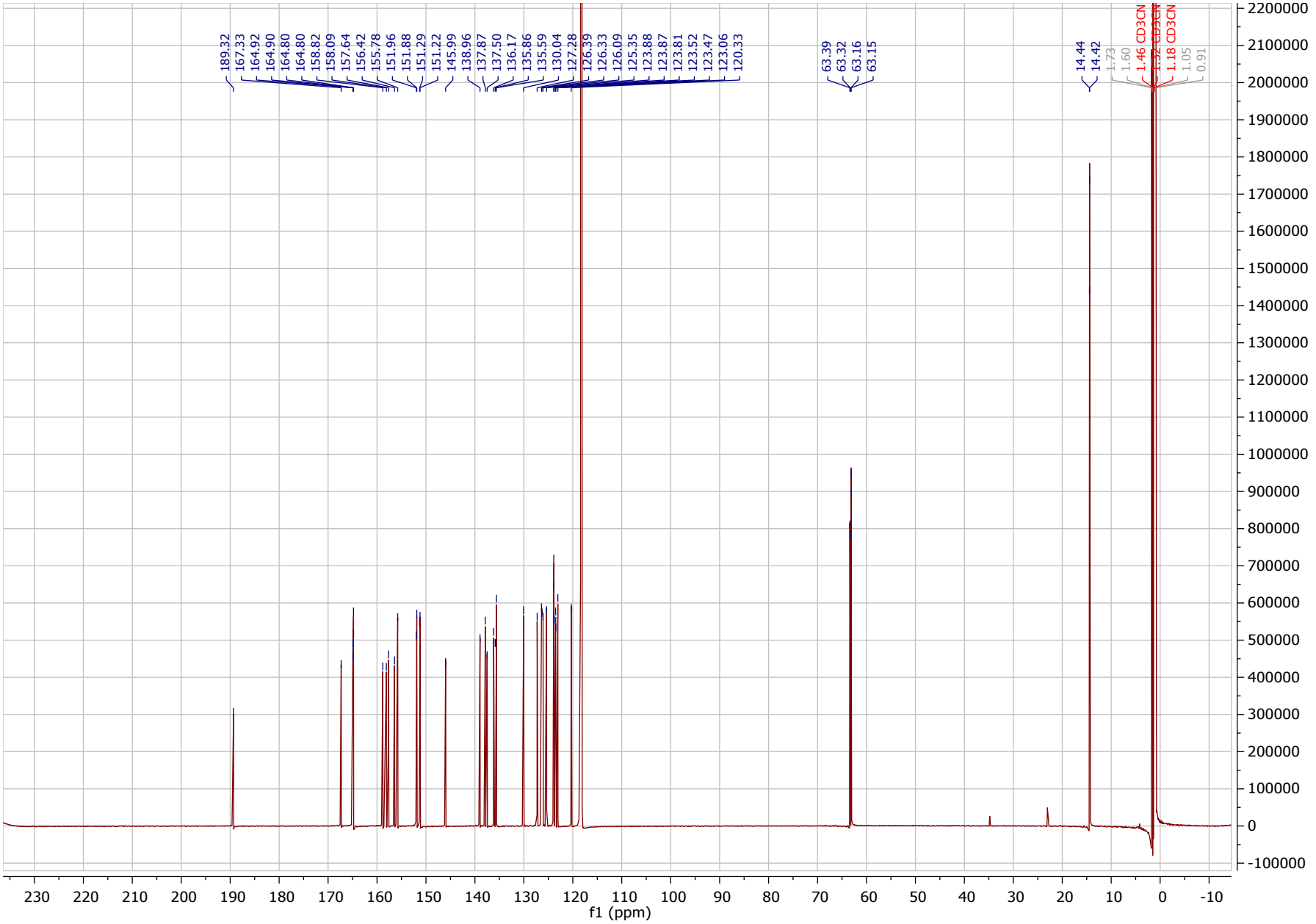

Figure S19. ^{13}C NMR spectrum of compound 4-Et. CD_3CN, 151 MHz.

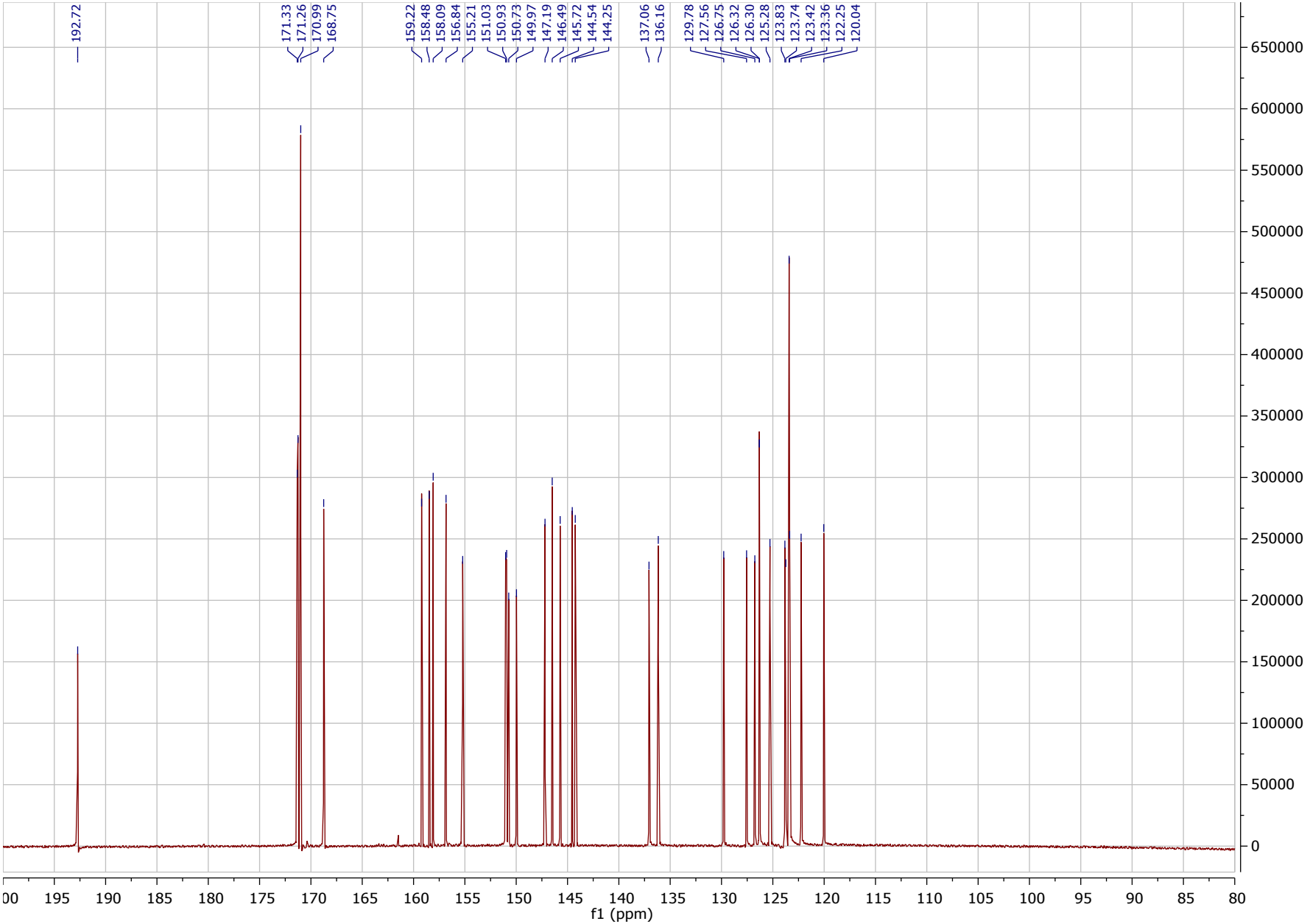

Figure S20. ^{13}C NMR spectrum of compound 4-Na. CD_3OD, 151 MHz.

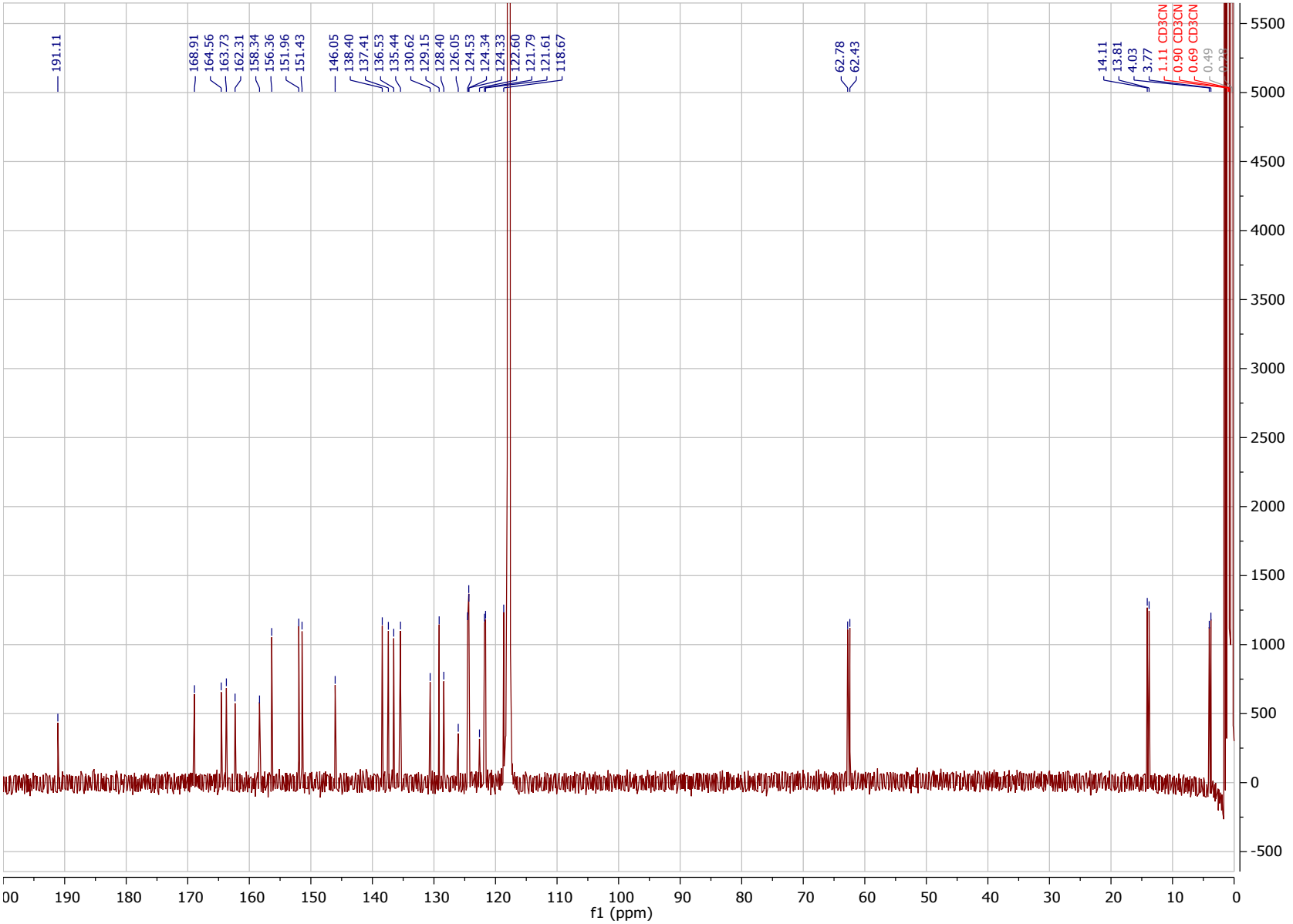

Figure S21. ^{13}C NMR spectrum of compound 6-Et. CD_3CN, 151 MHz.

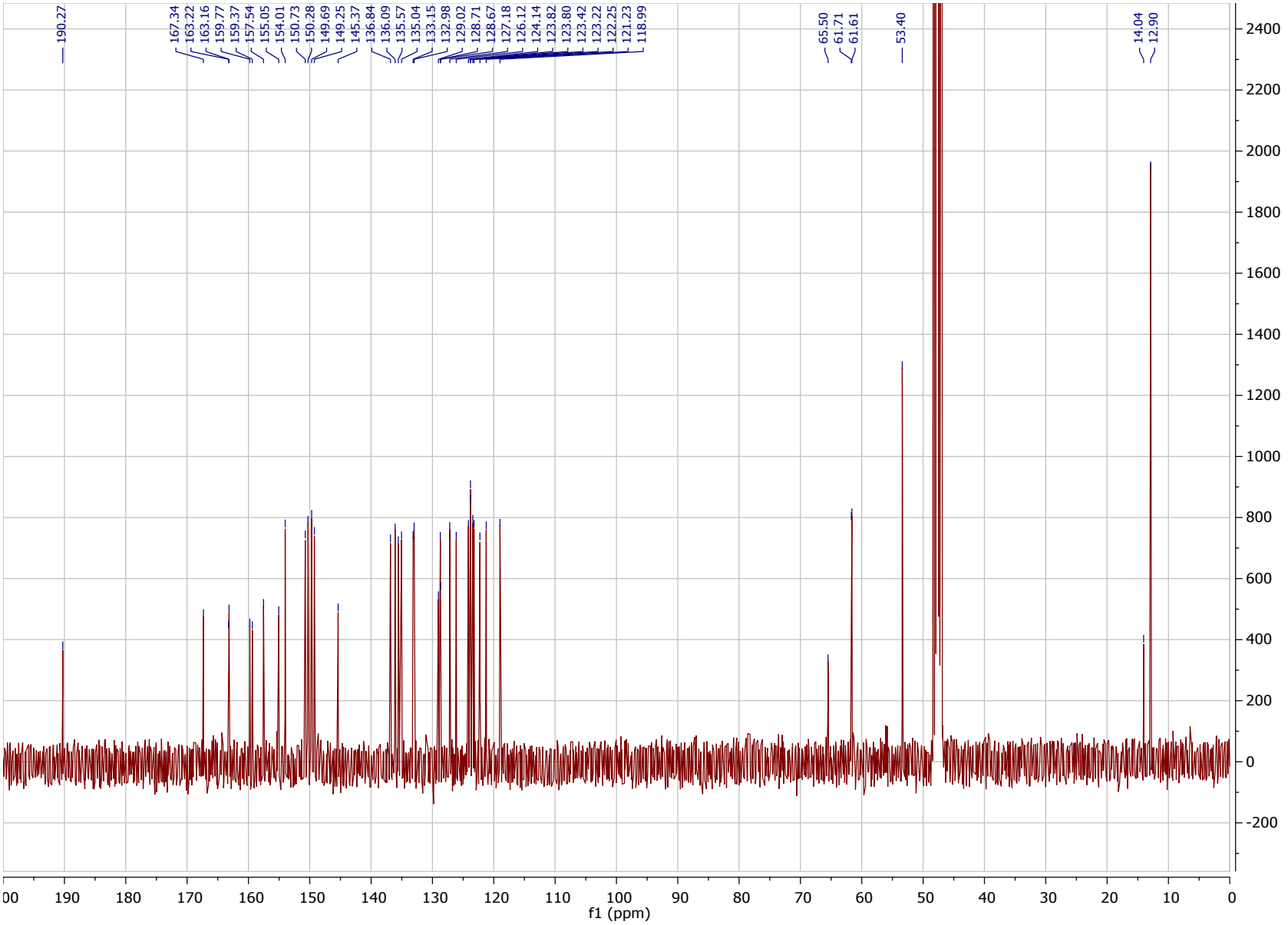

Figure S22. ^{13}C NMR spectrum of compound 7-Et. CD_3OD, 151 MHz.

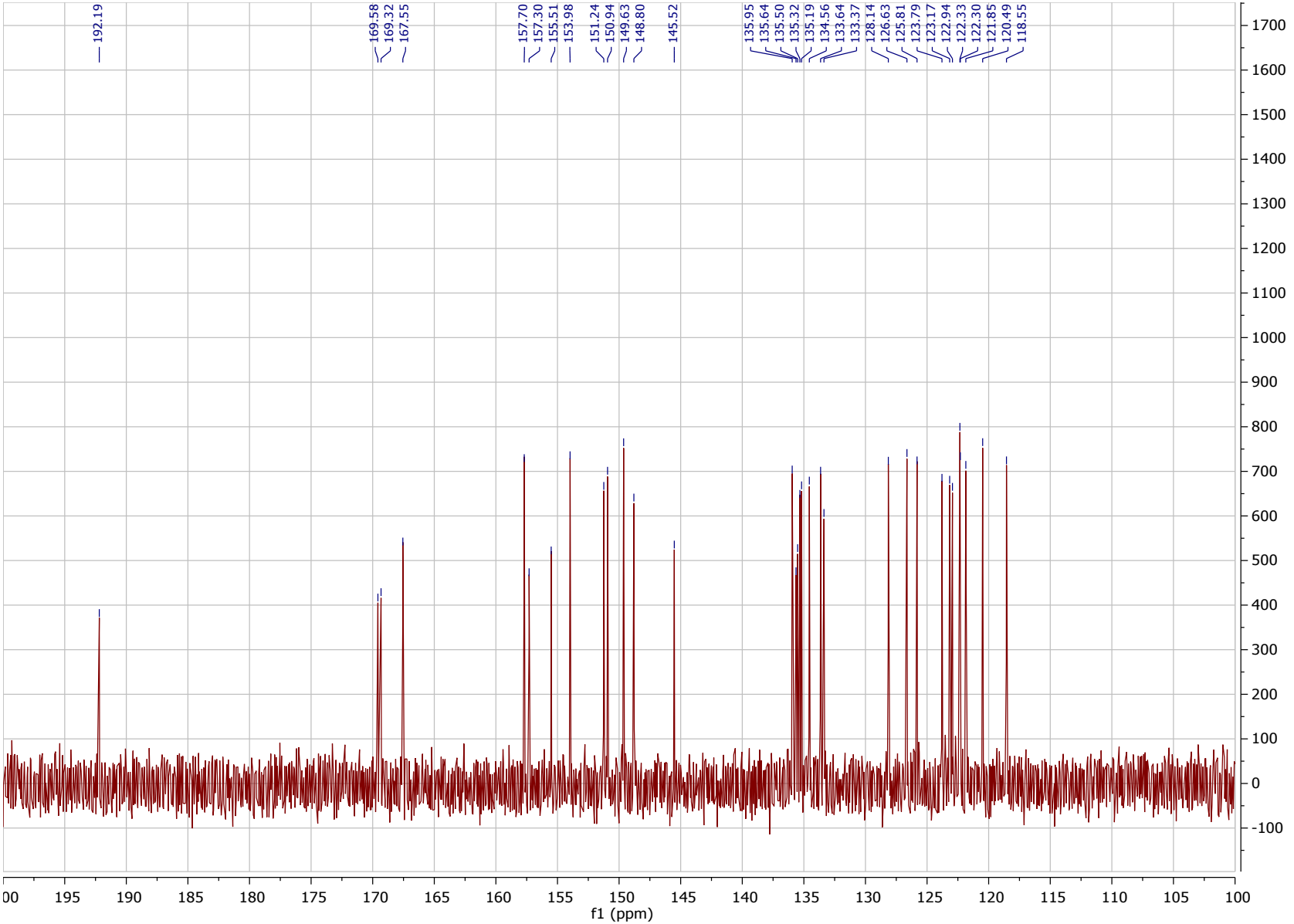

Figure S23. ^{13}C NMR spectrum of compound 7-Na. CD_3OD, 151 MHz.

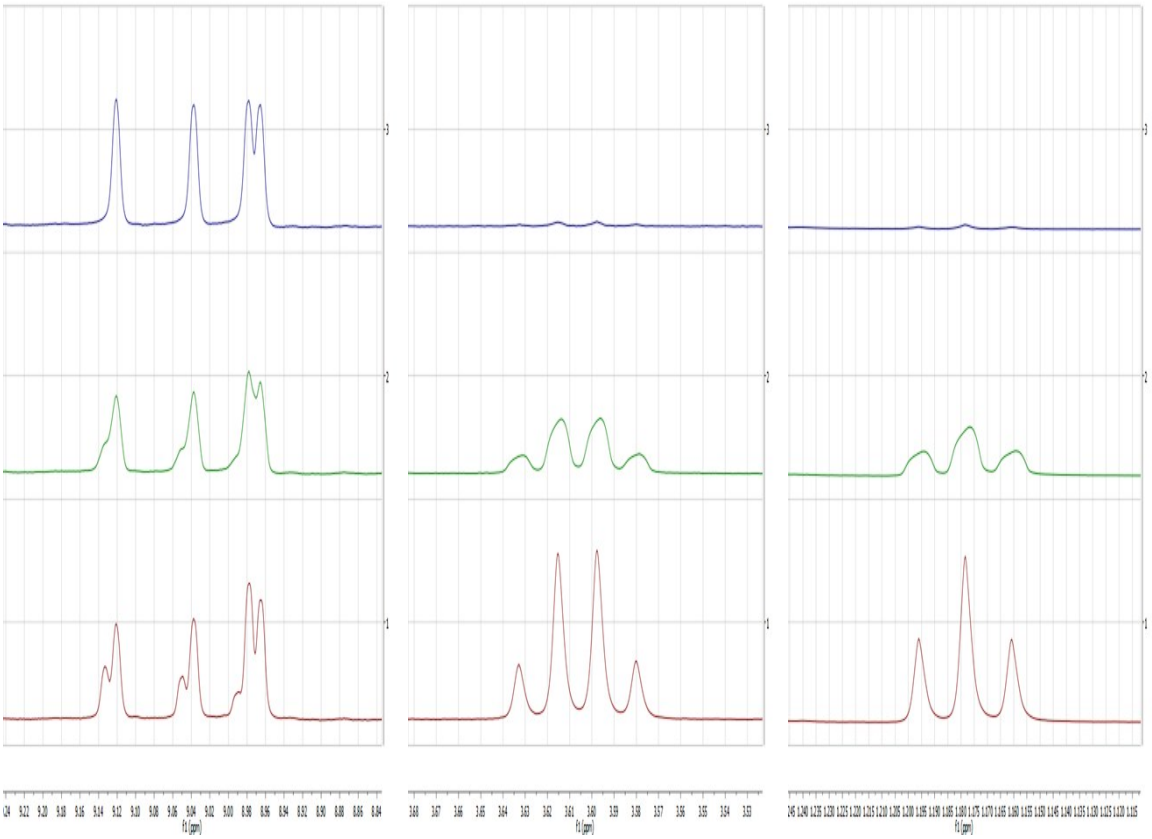

Figure S24. ^{1}H NMR spectra of compound 4-Et in CD_3OD that show transesterification over time. It is one day between the acquirement of the blue and green spectra and 6 days between the green and red spectra. The left panel shows part of the aromatic region of the spectrum of 4-Et and the middle and right panel show the quartet and triplet of the ethanol that is produced as a result of the transesterification.

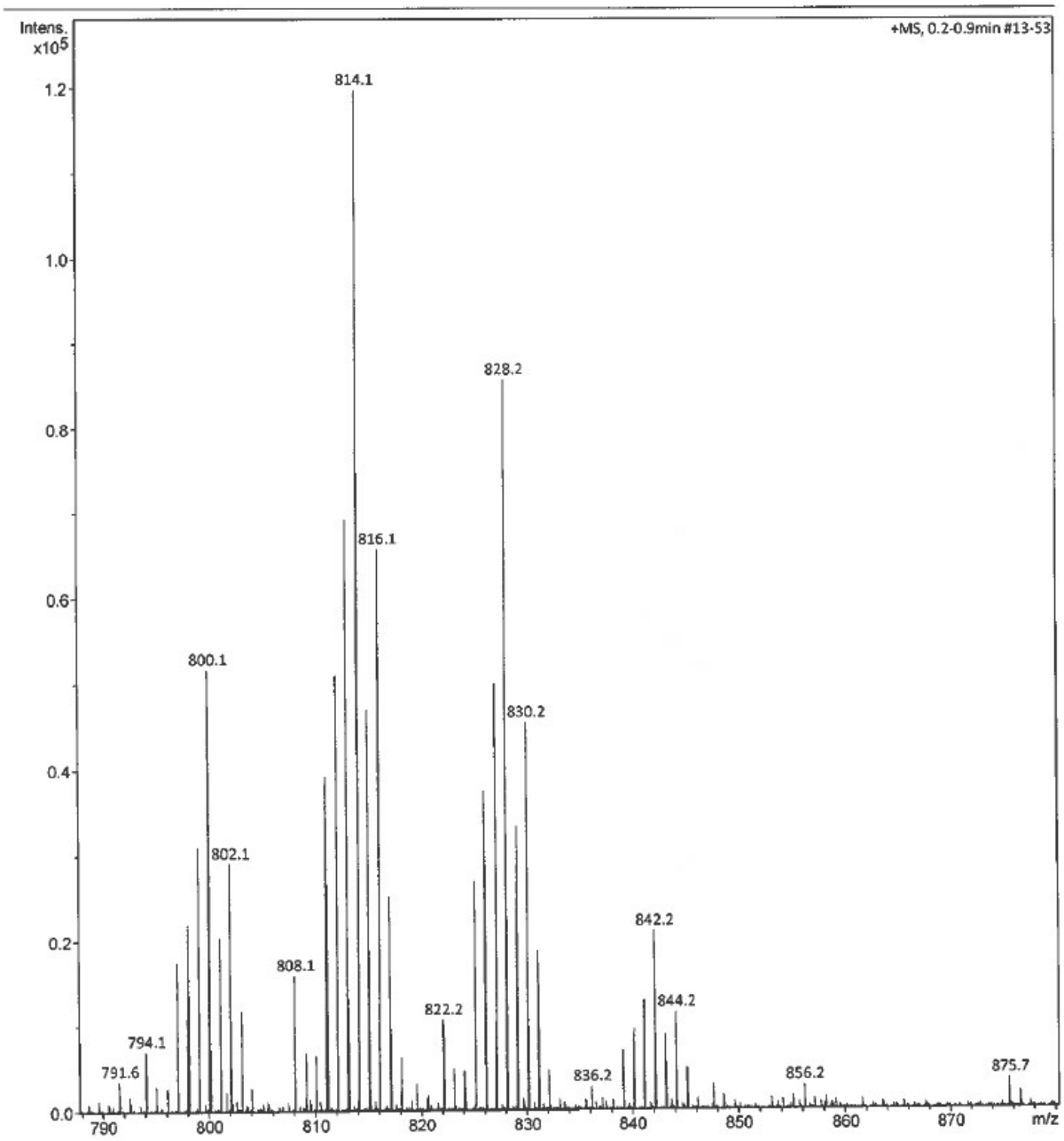

Figure S25. ESI-MS spectrum of compound 4-Et in CH_3OH that shows a distribution of the complex with different numbers of methyl ester groups as a result of transesterification: zero: m/z=856.2, one: m/z=842.2, two: m/z=828.2, three: m/z=814.1 and four: m/z=800.1.

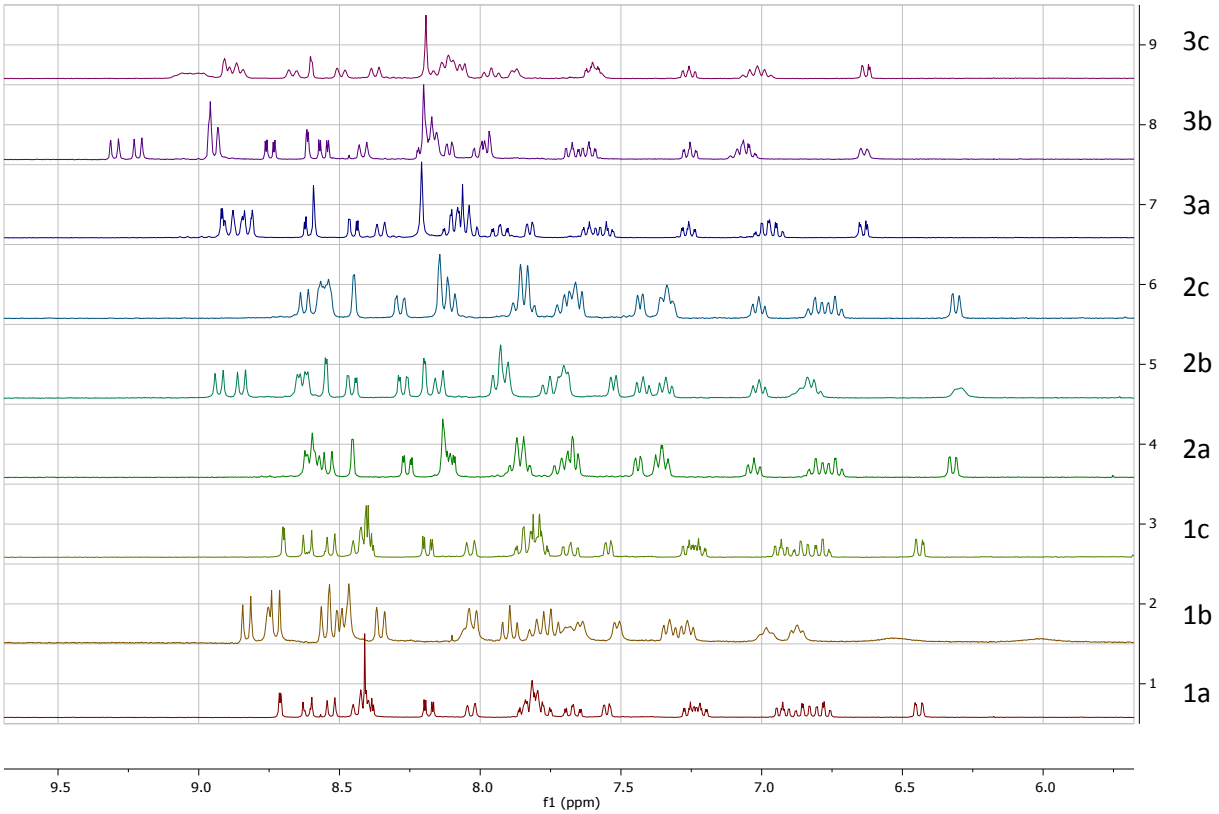

Figure S26. ^{1}H NMR spectra of compound 2-Na that show reversible protonation in three solvents: CD_3OD (1), DMSO (2) and DMF (3), each in pure solvent (a), with added 15 µl 1M HCl (b) and with consecutively added 15 µl 1M NaOH.

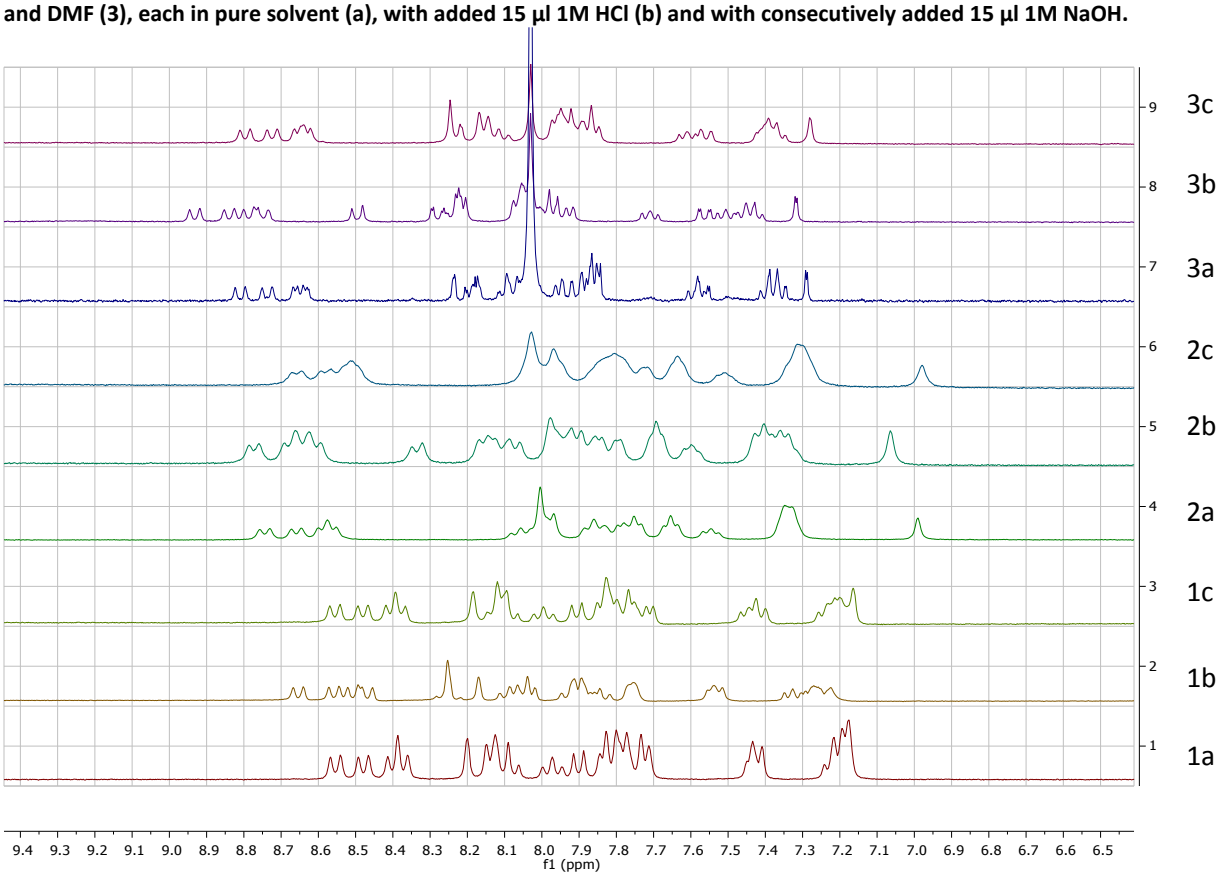

Figure S27. ^{1}H NMR spectra of compound 3-Na that show reversible protonation in three solvents: CD_3OD (1), DMSO (2) and DMF (3), each in pure solvent (a), with added 15 µl 1M HCl (b) and with consecutively added 15 µl 1M NaOH.

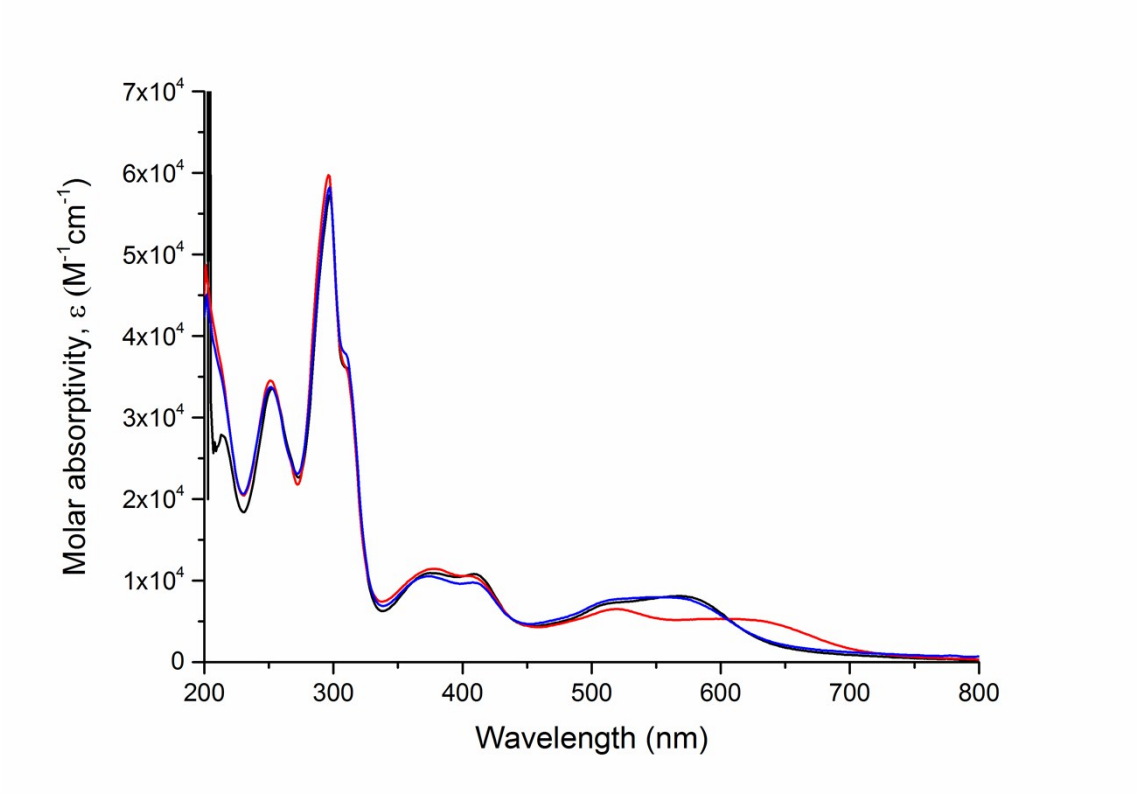

Figure S28. UV-Vis spectra of compound 2-Na that shows reversible protonation in CH_3OH. Black curve is in pure solvent, red curve is with added 150 µl 1M HCl (to 30 ml CH_3OH) and blue curve is with consecutively added 150 µl 1M NaOH. The concentration of metal complex is 3,9 x 10^{-5} mol/L.

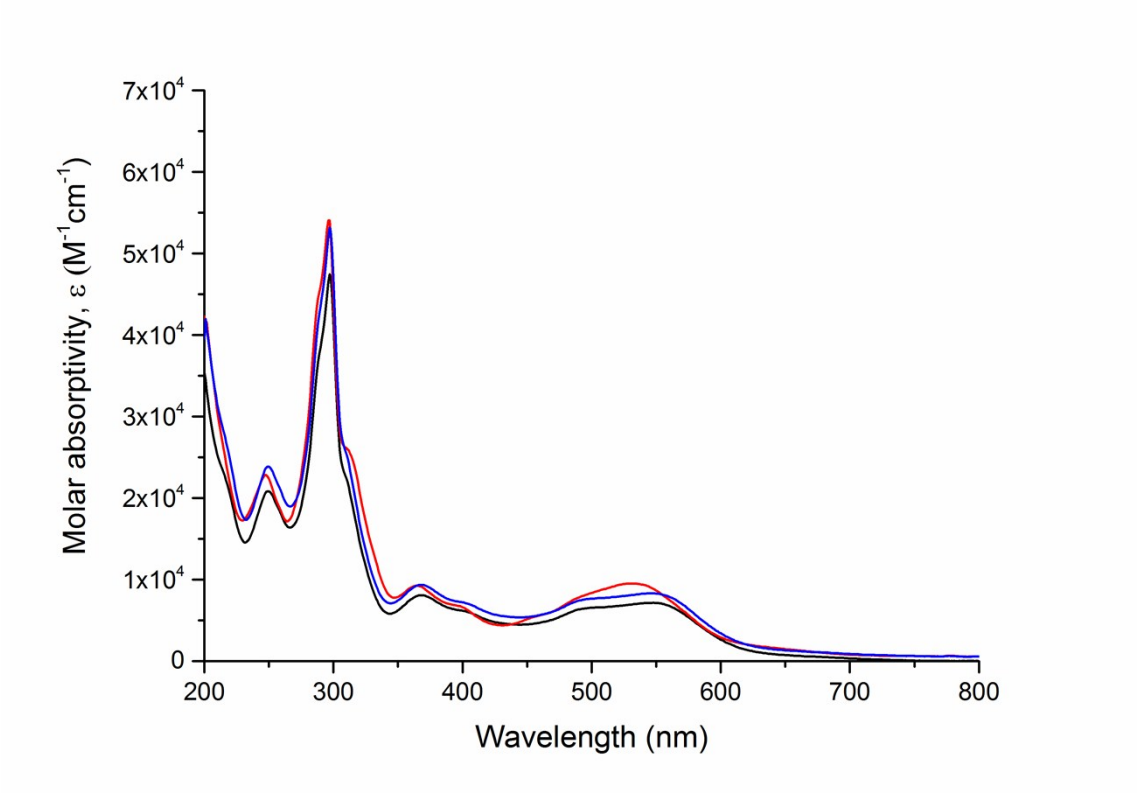

Figure S29. UV-Vis spectra of compound 3-Na that shows reversible protonation in CH_3OH. Black curve is in pure solvent, red curve is with added 150 µl 1M HCl (to 30 ml CH_3OH) and blue curve is with consecutively added 150 µl 1M NaOH. The concentration of metal complex is 3,9 x 10^{-5} mol/L.

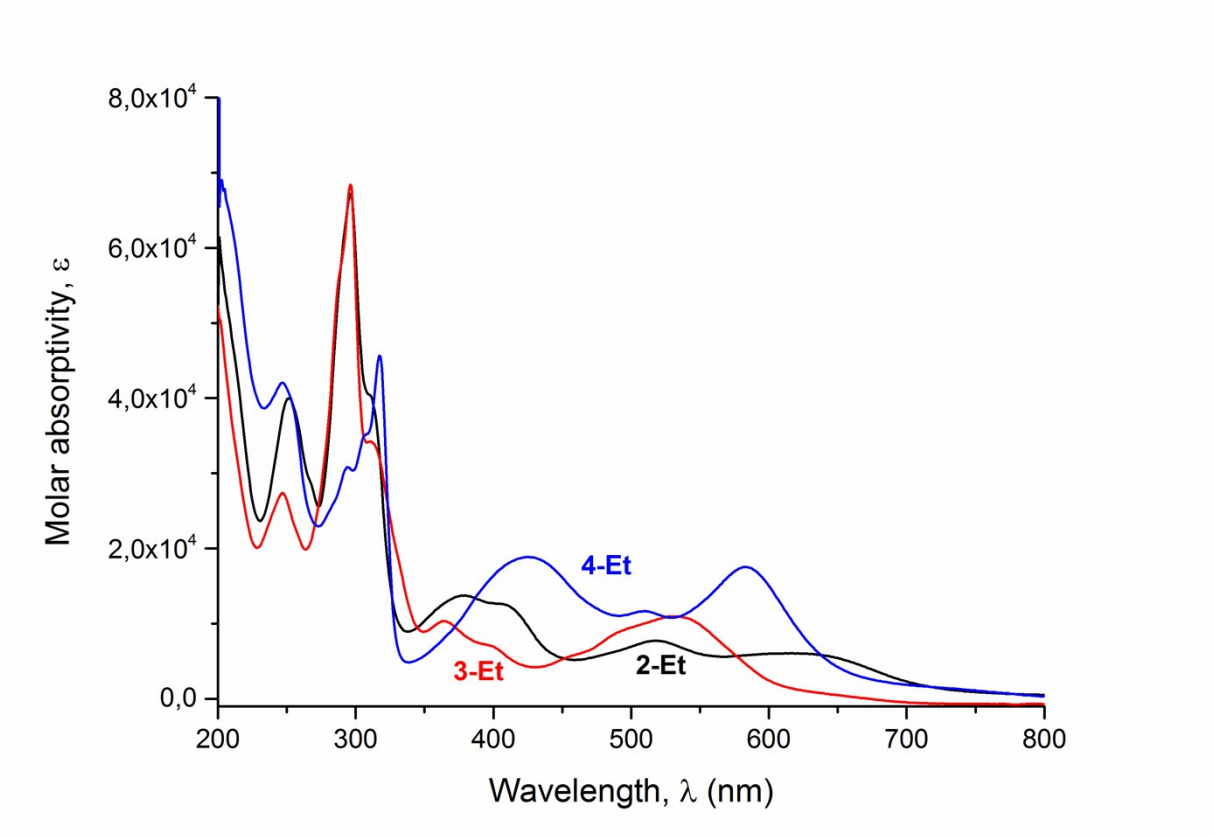

Figure S30. UV-Vis spectra of ester complexes 2-Et, 3-Et and 4-Et in CH_3OH.

X-Ray Crystallography

Table S1. Crystallographic data, data collection and refinement details for complexes $[Ru(ppy)(bpy)(MeCN)_2]PF_6$, 1-H, 2-Et, 2-Na, 3-Et, 3-Na, 6-Et and 7-Et

	[RU(PPY)(BPY)(MECN)$_2$]PF$_6$	**1-H**	**2-ET**	**2-NA**	**3-ET**	**3-NA**	**6-ET**	**7-ET**
CRYSTAL DATA								
CHEMICAL FORMULA	$C_{25}H_{22}N_5Ru{\cdot}F_6P{\cdot}C_2H_3N$	$2(C_{32}H_{22}N_6O_4Ru){\cdot}2(Cl)$	$2(C_{37}H_{32}N_5O_4Ru){\cdot}2(F_6P){\cdot}CO$	$C_{33}H_{22}N_5O_4Ru{\cdot}2(CH_4O)$	$2(C_{37}H_{32}N_5O_4Ru){\cdot}2(F_6P){\cdot}C_3H_6O$	$C_{35}H_{30}N_5NaO_6Ru{\cdot}CH_3O{\cdot}C_{1.5}O{\cdot}C_2H_3N$	$C_{31}H_{30}N_5O_4Ru{\cdot}F_6P$	$C_{37}H_{32}N_5O_4Ru{\cdot}CH_2Cl_2{\cdot}F_6P{\cdot}C_{2.5}$
M_R	679.57	1382.15	1741.44	717.71	1771.51	846.8	782.64	971.66
CRYSTAL SYSTEM, SPACE GROUP	Triclinic, P-1	Triclinic, P-1	Triclinic, P-1	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$	Triclinic, P-1	Monoclinic, P21/n	Triclinic, P1
TEMPERATURE (K)	100	100	100	100	100	100	273	102
A, B, C (Å)	9.5477 (10), 12.2940 (13), 12.7589 (13)	12.7453 (7), 13.6624 (7), 19.9377 (10)	11.3476 (7), 12.5085 (8), 13.5994 (9)	13.5773 (10), 12.7565 (9), 17.9162 (12)	15.5215 (8), 29.5909 (15), 18.0996 (10)	8.5931 (7), 12.6268 (11), 17.7433 (15)	12.8750 (12), 9.1042 (8), 27.598 (3)	9.259 (1), 12.8556 (14), 17.920 (2)
A, B, Γ (°)	102.363 (2), 107.081 (2), 94.071 (2)	97.029 (2), 99.656 (2), 94.114 (2)	82.510 (2), 67.804 (2), 81.017 (2)	90, 100.516 (2), 90	90, 92.509 (1), 90	93.898 (2), 96.346	90, 93.750 (2), 90	86.107 (2), 78.113

						(2), 92.495 (2)		(2), 88.160 (2)
V (Å^3)	1383.9 (3)	3381.7 (3)	1760.0 (2)	3050.9 (4)	8305.1 (8)	1906.5 (3)	3228.0 (5)	2082.1 (4)
Z	2	2	1	4	4	2	4	2
RADIATION TYPE	Mo Kα	Mo Kα	Mo Kα	Mo Kα	Mo Kα	Mo Kα	Mo Kα	Mo Kα
M (MM^{-1})	0.69	0.59	0.57	0.57	0.49	0.48	0.62	0.62
CRYSTAL SIZE (MM)	0.23 × 0.12 × 0.09	0.30 × 0.10 × 0.05	0.20 × 0.18 × 0.13	0.31 × 0.12 × 0.07	0.28 × 0.08 × 0.06	0.21 × 0.18 × 0.12	0.05 × 0.05 × 0.05	0.37 × 0.15 × 0.03
DATA COLLECTION								
DIFFRACTOMETER	Bruker D8 venture, cmos detector	Bruker d8 venture, cmos detector	Bruker d8 venture, cmos detector	Bruker d8 venture, cmos detector	Bruker d8 venture, cmos detector	Bruker d8 venture, cmos detector	Bruker d8 venture, cmos detector	Bruker d8 venture, cmos detector
ABSORPTION CORRECTION	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan
TMIN, TMAX	0.658, 0.746	0.702, 0.745	0.709, 0.745	0.654, 0.746	0.684, 0.746	0.680, 0.746	0.688, 0.746	0.598, 0.746
NO. OF MEASURED, INDEPENDENT AND OBSERVED [I > 2Σ(I)] REFLECTIONS	45870, 9149, 8722	115607, 12420, 10055	45114, 7179, 6093	28996, 7597, 6141	178386, 25404, 21223	28651, 10644, 9700	42287, 8036, 6719	23690, 9332, 7466
RINT	0.022	0.049	0.041	0.035	0.04	0.023	0.051	0.049
(SIN Θ/Λ)$_{MAX}$ (Å^{-1})	0.735	0.604	0.625	0.669	0.715	0.695	0.668	0.646
REFINEMENT								
R[F^2 > 2Σ(F^2)], WR(F^2), S	0.024, 0.059, 1.08	0.047, 0.095, 1.04	0.029, 0.062, 1.06	0.048, 0.144, 1.04	0.035, 0.092, 1.06	0.037, 0.101, 1.12	0.070, 0.155, 1.14	0.052, 0.128, 1.03
NO. OF REFLECTIONS	9149	12420	7179	7597	25404	10644	8036	9332
NO. OF PARAMETERS	373	902	545	429	1053	524	543	437
NO. OF RESTRAINTS	0	30	0	0	0	6	0	0
ΔP$_{MAX}$, ΔP$_{MIN}$ (E Å^{-3})	1.92, −1.13	0.85, −0.87	0.37, −0.48	1.47, −1.18	0.92, −0.78	1.04, −0.93	2.34, −1.69	1.17, −1.33

The crystal used to determine the structure of **1-H** was twinned by reticular merohedry. The reflections were sorted manually and the twin rotation matrix was found to be $\begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & -1 & 0 \\ -\frac{3}{2} & 0 & -\frac{1}{2} \end{pmatrix}$. The crystals of **1-H** and **3-Et** contains disordered solvent molecules which were not possible to include in the crystal structure in a meaningful way by a restrained solvent disorder model. The contribution of the disordered solvent to the diffraction data was calculated using SQUEEZE[1] for these compounds.

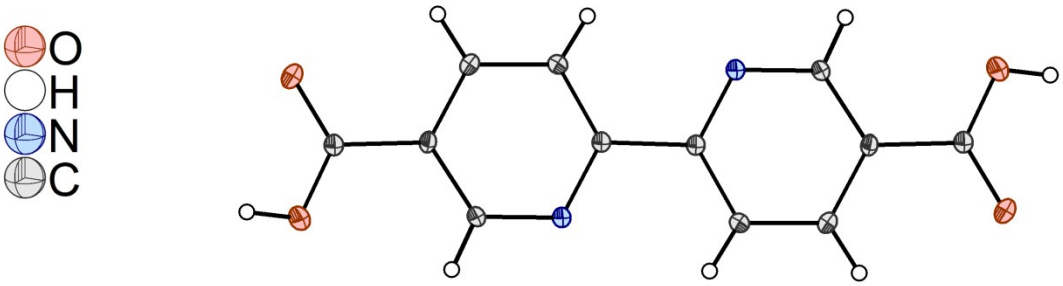

Figure S31. Molecular structure of the ligand 2,2'-bipyridine-5,5'-dicarboxylic acid, determined by single-crystal X-ray diffraction. Ellipsoids are shown at 50 % probability.

Table S2. Crystallographic data, data collection and refinement details for 2,2'-bipyridine-5,5'-dicarboxylic acid

Crystal data	
Chemical formula	$C_{12}H_8N_2O_4$
Mr	244,2
Crystal system, space group	Triclinic, P
Temperature (K)	100
a, b, c (Å)	4.9956 (7), 7.0437 (9), 7.2755 (10)
α, β, γ (°)	85.544 (3), 80.042 (3), 77.090 (3)
V (Å^3)	245.57 (6)
Z	1
Radiation type	Mo Kα
μ (mm−1)	0,13
Crystal size (mm)	0.19 × 0.14 × 0.08
Data collection	
Diffractometer	Bruker Venture
	diffractometer
Absorption correction	Multi-scan
	SADABS2014/3 (Bruker,2014) was used for absorption correction. wR2(int) was 0.0599 before and 0.0296 after correction. The Ratio of minimum to maximum transmission is 0.9395. The λ/2 correction factor is Not present.
Tmin, Tmax	0.030, 0.060
No. of measured, independent and observed [I > 2σ(I)] reflections	6483, 1227, 1041
Rint	0,021
(sin θ/λ)max (Å−1)	0,67
Refinement	

R[F2 > 2σ(F2)], wR(F2), S	0.038, 0.118, 1.10
No. of reflections	1227
No. of parameters	95
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρmax, Δρmin (e Å−3)	0.51, −0.22

Computational Section

Computational Details

Structures were fully optimized with no geometry or symmetry constraints at the DFT level with the Gaussian09 program.[2] The M11L functional[3] including dispersion was selected upon method benchmarking, in which theoretical and experimental UV-Vis spectra were systematically compared (*vide infra*). Electronic excitations were determined by means of TD-DFT(M11L) single-point calculations on the DFT(M11L)-optimized geometries.[4] The absorption bands were convoluted by using Gaussian peak shapes with a band width at half-height of 3000.0 cm^{-1}.[5]5 The lighter elements (C, N, O, Na and H) were described with the all-electron 6-311G** basis set,[6] whereas the heaviest (Ru) was described with the ECP-adapted LANL2TZ(f) basis set[7] accounting for relativistic effects (f coefficient = 1.235). All these basis sets are of triple-ζ quality and include polarization functions. The ultrafine pruned (99,590) grid was used for higher numerical accuracy. Solvent effects were introduced both in the DFT optimizations and TD-DFT single-points by using the continuum SMD model[8] for methanol. The relative stability of the different isomers of complex **2-Na** in the Na^+ ion-pair form were assessed by comparing their absolute free energies at the DFT(M11L) level, which were derived from thermochemistry calculations on the translational, rotational and vibrational modes. These calculations were also used to confirm that the stationary points located in the potential energy hypersurface were energy minima; *i.e.*, all their vibrational frequencies are real. The molecular orbitals involved in the electronic excitations were plotted with the GaussView software (version 5).

Functional Benchmarking

The experimental UV-Vis spectrum of complex **1-Na** was used as reference to benchmark the functional used in the TD-DFT/SMD(methanol) calculations. Both pure (M11L, PBE[9] and lc-ωPBE[10]) and hybrid (M11[11], PBE0,[12] M06-2X,[13] B3LYP,[14] CAM-B3LYP,[15] ωB97xd[16]) functionals were considered. The data plotted in Figure S32 shows that the UV-Vis spectra predicted by the lc-ωPBE, M11 and M06-2X functionals are strongly blue-shifted compared to the experimental. Further, the spectra appear compressed; *e.g.*, the *ca.* 150 nm separation between the UV and Vis absorption peaks in the experiment is reduced to *ca.* 50 nm in the TD-DFT(M06-2X) calculation. Figure S33 shows that the TD-DFT spectra become closer to the experimental with the CAM-B3LYP, PBE0 and ωB97xd functionals. However, with the closest functional, the PBE0, the Vis adsorption band is still blue-shifted by *ca.* 50 nm with

respect to the experimental. The B3LYP functional shows a similar behavior (Figure S34), which has been also observed with other ruthenium complexes supported by bpy ligands.[17,18] The deviation in the Vis region is reduced to almost zero with the spectrum predicted at the TD-DFT(M11L) level; the experimental and TD-DFT(M11L) adsorption maxima are at 456 and 457 nm, respectively. Since absorption in the visible region of the spectrum is the most relevant, the M11L functional was selected to study all other species. This functional also predicts accurate geometries, as shown by the low RMSD values relative to experimental X-Ray diffraction structures: 0.024, 0.034 and 0.015 Å for the metal-ligand distances, *i.e.* Ru–N and Ru–C, in **2-Et**, **3-Na** and $[Ru(bpy)(ppy)(MeCN)_2]^+$, respectively. The difficulty of predicting the UV-Vis spectra can be ascribed to the presence of the carboxylate groups and their dynamic interactions with the solvent, which are not fully included in the TD-DFT model. In line with this, the spectrum difference recorded in acetonitrile between $[Ru(bpy)_3]^{2+}$ and $[Ru(bpy)_2(ppy)]^+$, which do not contain carboxylate groups, was better reproduced at the TD-DFT(M11L); *i.e.*, the single absorption band of $[Ru(bpy)_3]^{2+}$ in the 400-500 nm range (most intense transition predicted at λ = 450 nm) splits in two with $[Ru(bpy)_2(ppy)]^+$, with absorption in the 300-400nm and 500-600 nm ranges (most intense transitions predicted at λ = 377 and 535 nm).

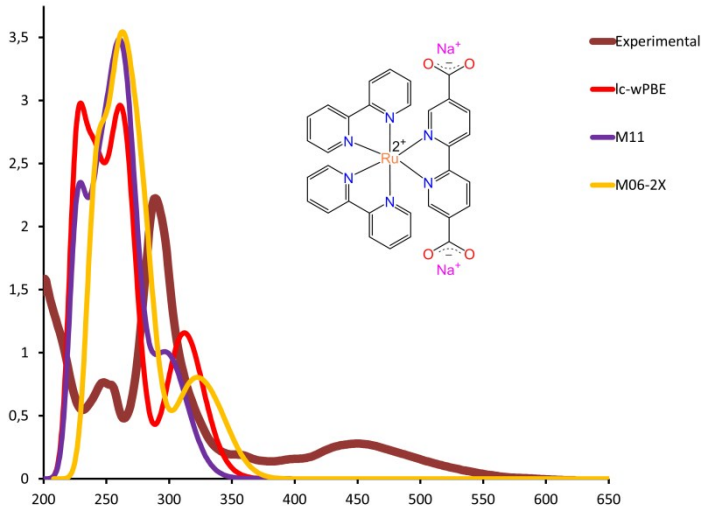

Figure S32. Experimental and TD-DFT (lc-ωPBE, M11 and M06-2X) UV-Vis spectra of complex 1-Na in methanol showing absorbance versus λ in nm.

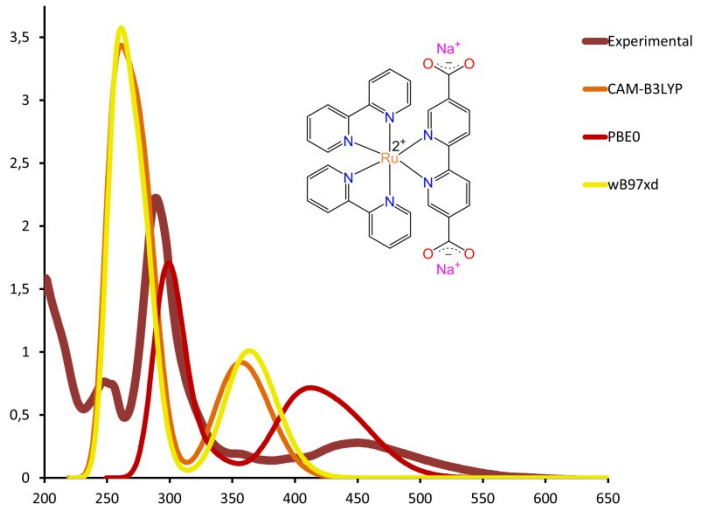

Figure S33. Experimental and TD-DFT (CAM-B3LYP, PBE0 and ωB97xd) UV-Vis spectra of complex 1-Na in methanol showing absorbance versus λ in nm.

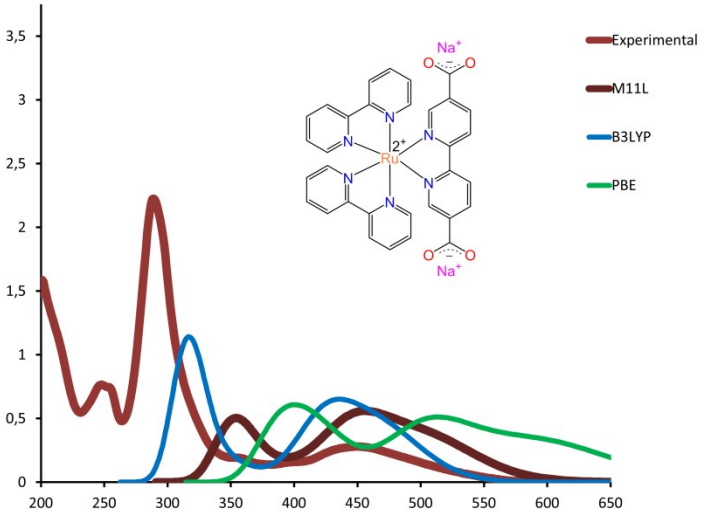

Figure S34. Experimental and TD-DFT (M11L, B3LYP and PBE) UV-Vis spectra of complex 1-Na in methanol showing absorbance versus λ in nm.

C-trans-bpy and C-trans-bpydc isomers of 2-Na

The difference between the UV-Vis spectra predicted by TD-DFT calculations for the *C-trans-bpy* and *C-trans-bpydc* isomers of **2-Na** (Figure S35) shows that the *trans* influence has a significant influence on the electronic structure of these complexes. Upon isomerization,

the absorbance peak of the *C-trans-bpy* isomer at 631 nm is blue-shifted to 604 nm in the *C-trans-bpydc*. This peak merges with the one at 527 nm, yielding a single broad band (Figure 6). These absorbances are associated with the HOMO-1 → LUMO electronic transition in the *C-trans-bpy* isomer and the HOMO-2 → LUMO in the *C-trans-bpydc* (Table 3). These three frontier orbitals have very similar shapes. However, whereas the LUMO has the same energy in both cases, -3.2 eV, the HOMO-1 of *C-trans-bpy* is 0.1 eV higher than the HOMO-2 of *C-trans-bpydc*, which yields the blue-shifted absorption in the latter isomer. This energy difference is due to the out-of-phase interaction between the metal *d* orbital bisecting the Ru,N(*bpydc*),N(*bpydc*) plane and the π system of one aromatic ring of the ppy ligand (see Figure S35). This interaction is stronger and thus more destabilizing in the *C-trans-bpy* isomer than in the *C-trans-bpydc* due to the higher negative charge of the aromatic ring, which, formally, is $C_6H_4^-$ in the former and C_5NH_4 in the latter.

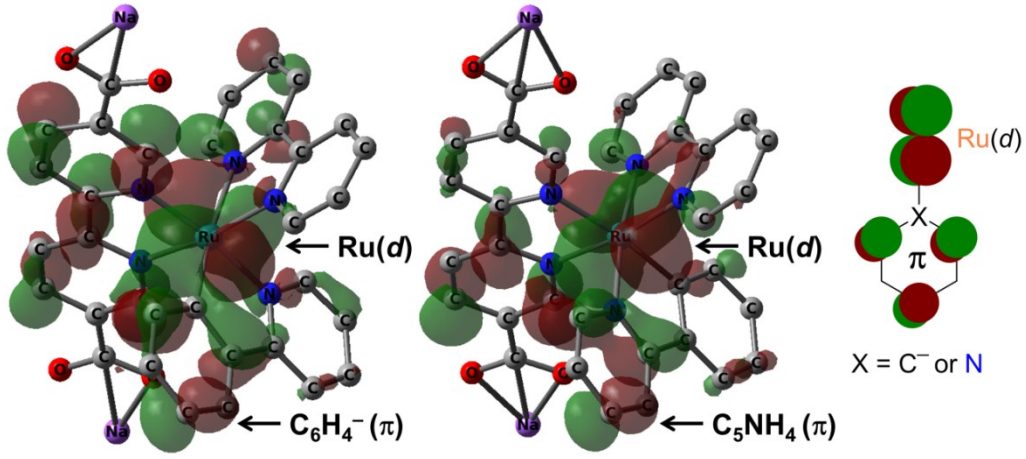

Figure S35. HOMO-1 of 2-Na *C-trans-bpy* (left), HOMO-2 of 2-Na *C-trans-bpydc* (middle) and diagram showing the interaction between the Ru *d* and aromatic ring π orbitals (top view perpendicular to the π system; right). Orbitals shown at isovalue = 0.02 *a.u.*

Optimized geometries (Å) and energies (potential, E, and free, G, both in h) at the DFT(M11L) level

1-Na E = –2280.817464

Ru	-0.00059200	0.40736800	0.00285400
N	0.47131000	0.53601100	1.99458400
O	5.61074300	-3.01875800	-0.51331600
N	-1.28273800	-1.18540100	0.12909600
O	-5.61605000	-3.01454500	0.50244000
N	1.28215400	-1.18588500	-0.11137700
N	-1.42403800	1.87991900	-0.01935400
N	1.42268800	1.88036300	0.01270000
N	-0.47090600	0.52041900	-1.99017000
C	1.40574000	1.44174800	2.32857200
C	-0.72487000	-2.40843900	0.07837700
C	-2.59858100	-1.09135000	0.24603200
H	-3.01662800	-0.08327700	0.28768900
C	2.86109200	-3.44559700	-0.23792300
H	3.49144500	-4.33419900	-0.29021400
C	-1.93705000	2.19913200	-1.21877000
C	0.72527200	-2.40857700	-0.04568500
C	1.80425600	1.61792700	3.64169100
H	2.56233300	2.35698600	3.89321400
C	-0.07261300	-0.20076600	2.95542900
H	-0.83137700	-0.92030400	2.64125000
C	1.49716600	-3.55556800	-0.10696600
H	1.03033300	-4.53723400	-0.05449400
C	1.93991100	2.20557400	1.20880100
C	-2.86102000	-3.44476800	0.27060400
H	-3.49140900	-4.33296600	0.32721500
C	-3.43435200	-2.18704400	0.31994400
C	3.43346400	-2.18815700	-0.30518400
C	-1.86675000	2.52162800	1.05446500
H	-1.42846700	2.22243400	2.00861100
C	0.07306600	-0.22445500	-2.94480800
H	0.82908200	-0.94397700	-2.62405000
C	1.86174600	2.51710600	-1.06568500
H	1.41921200	2.21481600	-2.01693900
C	0.27488400	-0.07825200	4.28077000
H	-0.20957800	-0.71140300	5.02277200
C	-1.49617200	-3.55521900	0.14944900
H	-1.02833500	-4.53710300	0.10953700
C	4.91241600	-1.99897100	-0.45616400
C	-2.82892600	3.50284700	0.99624300
H	-3.15248500	3.99192300	1.91401600
C	2.59764100	-1.09219800	-0.23552100
H	3.01476800	-0.08438200	-0.29119100
C	-1.40179900	1.42691500	-2.33241800
O	5.33953800	-0.83764300	-0.51308200
C	-4.91472800	-1.99645500	0.45110000
C	-2.90593700	3.17761700	-1.35236600
H	-3.31027600	3.42270600	-2.33259800
C	-3.35780400	3.83906500	-0.23313500
H	-4.12200100	4.61197700	-0.32181900
C	1.23346200	0.85027300	4.63090400
H	1.53618300	0.97877000	5.67066400
C	2.91103600	3.18284400	1.33413200
H	3.31976400	3.43184000	2.31159700
C	-0.27129500	-0.10988500	-4.27172600
H	0.21275000	-0.74956300	-5.00837400

C	2.82558500	3.49723300	-1.01545700
H	3.14598900	3.98200600	-1.93660500
C	3.36029300	3.83774900	0.21018600
H	4.12650200	4.60943900	0.29238400
O	-5.34039700	-0.83391300	0.49841700
C	-1.22613200	0.81930200	-4.63034500
H	-1.52588900	0.94166800	-5.67166100
C	-1.79681900	1.59553400	-3.64766700
H	-2.55204600	2.33527300	-3.90568900
Na	7.47490300	-1.67479900	-0.71447800
Na	-7.48098000	-1.66606600	0.67846000

2-Et

Ru	-0.08190700	0.50275300	0.00108600
O	5.76343200	-2.48582600	0.08626300
N	0.30159000	0.59591700	-2.03131900
N	-1.25497600	-1.29766900	-0.02780400
N	-0.44386500	0.69247000	1.99527900
N	1.31771700	-1.00668300	0.08016200
O	-5.36887200	-3.62173100	0.02934100
N	-1.56777500	1.88906400	0.03337400
C	1.22383700	2.03088400	-0.06658600
O	5.36248400	-0.29993400	0.19114700
C	-2.00685100	2.27996800	1.24408000
C	0.88270900	-2.28407500	0.03347900
C	-1.37206300	1.59708100	2.35800500
C	1.69929100	2.35643700	-1.35305700
C	1.71173600	2.79218400	0.99205300
H	1.38250900	2.58488500	2.01560600
C	-2.09171900	2.47091900	-1.04144800
H	-1.69545400	2.13419700	-2.00085900
C	1.18041200	1.54051500	-2.42913400
C	-2.98431900	3.25030900	1.38228400
H	-3.32061800	3.55061600	2.37278700
C	-0.56522800	-2.44778400	0.01423400
C	-1.66739500	1.83797600	3.68916000
H	-2.41880000	2.57788300	3.95802200
C	-3.28511100	-2.54074400	-0.00508600
C	-1.20361700	-3.67979100	0.04555100
H	-0.62928000	-4.60301400	0.08631400
C	2.62266700	3.81360600	0.79407900
H	2.98880500	4.38841700	1.64815600
C	-3.06387700	3.43989100	-0.97571900
H	-3.44712300	3.87782900	-1.89597700
C	3.56200400	-1.81404200	0.09688000
C	-2.57761600	-1.35576100	-0.03466500
H	-3.10191700	-0.39715200	-0.07009600
C	0.18732900	0.02342400	2.95535900
H	0.93847200	-0.69262400	2.61636800
C	1.50959500	1.66612400	-3.77395100
H	2.22016100	2.43037400	-4.08320000
C	1.76616700	-3.35142200	0.01310900
H	1.38988100	-4.37111500	-0.03458500
C	-3.52292300	3.84076100	0.26374700
H	-4.28876800	4.61040600	0.35760800
C	-0.23566400	-0.20827000	-2.94157300
H	-0.94083400	-0.95083200	-2.55960400
C	2.61655000	3.38422800	-1.54984300
H	2.98290100	3.62509100	-2.55029600
C	-1.00370900	1.14344300	4.67248800
H	-1.22251200	1.32672100	5.72425700

C	2.62877500	-0.79751000	0.11146000
H	2.96197300	0.24260000	0.15050400
C	4.99203900	-1.42655400	0.13324500
C	-0.05530100	0.21273800	4.29429400
H	0.50290600	-0.36541000	5.02895400
O	-5.29296100	-1.40019900	-0.05725800
C	3.12033000	-3.12459100	0.04297300
H	3.83382500	-3.94749500	0.02350900
C	3.07777600	4.11316800	-0.47861800
H	3.79834000	4.91653800	-0.63151600
C	0.04648500	-0.13239500	-4.28381100
H	-0.43045900	-0.82044200	-4.97932500
C	-4.76427300	-2.60095900	-0.01048800
C	0.94374200	0.83178400	-4.70590000
H	1.19964900	0.92972100	-5.76183100
C	-2.57490100	-3.72916500	0.03461600
H	-3.12224100	-4.67239200	0.06061600
C	7.64815300	-2.00217800	1.50881300
H	7.40762900	-2.85968900	2.15011500
H	7.20981500	-1.09758400	1.94701900
H	8.73805500	-1.87871700	1.50949200
C	7.16298900	-2.21879400	0.11237100
H	7.36574700	-1.34878400	-0.52894900
H	7.61223300	-3.10895300	-0.34623800
C	-6.71763100	-1.36862100	-0.06640700
H	-6.96382400	-0.36549500	0.30532100
H	-7.09001900	-2.11316300	0.65203400
C	-7.25865200	-1.60565200	-1.43881000
H	-7.02867200	-2.61916100	-1.78804300
H	-6.85050200	-0.88273200	-2.15679200
H	-8.34986100	-1.49461500	-1.43402700

2-Na *C-trans-to-bpy* E = –2264.291050; G = –2263.882415

Ru	0.01342200	0.38611400	0.01575800
N	-0.37442000	0.63501200	-2.07457300
O	-5.59449000	-3.04039800	0.42673600
N	1.28925500	-1.18929700	-0.13057300
O	5.63635800	-2.98948200	-0.53577300
N	-1.26262300	-1.19824200	0.04826400
N	1.44338700	1.86969200	0.17435300
N	-1.41475600	1.87104800	-0.04370200
C	-1.30071600	1.54863400	-2.39145900
C	0.73726100	-2.41853800	-0.14776800
C	2.60881900	-1.09162000	-0.22812000
H	3.02509000	-0.08238100	-0.20631800
C	-2.84565400	-3.46802800	0.13616500
H	-3.47637700	-4.35680600	0.17523000
C	1.86858300	2.16801200	1.41965500
C	-0.70931100	-2.42417300	-0.03400600
C	-1.66598600	1.78891000	-3.70674300
H	-2.42450700	2.53109300	-3.94861700
C	0.20302700	-0.04643400	-3.05396300
H	0.95863700	-0.77657900	-2.74913500
C	-1.48244800	-3.57285000	0.00560300
H	-1.01240100	-4.55257700	-0.06096300
C	-1.87549300	2.25394400	-1.24963100
C	2.87812700	-3.44263200	-0.37456300
H	3.51144400	-4.32506100	-0.47192100
C	3.44688400	-2.17989700	-0.35248600
C	-3.41628600	-2.20849900	0.22161600
C	1.95188300	2.53847600	-0.85423200

H	1.58164700	2.25148200	-1.84157600
C	-0.27299700	-0.39495200	2.98194600
H	-1.00932900	-1.15405200	2.69303800
C	-1.90967900	2.47420800	1.03398400
H	-1.51478900	2.13185400	1.99210200
C	-0.10274400	0.13550500	-4.38339800
H	0.40744600	-0.45586400	-5.14300200
C	1.51343300	-3.55916000	-0.27173900
H	1.04487700	-4.54174700	-0.28719300
C	-4.89304900	-2.02090000	0.37718400
C	2.89499200	3.52983400	-0.72144900
H	3.27291500	4.03859200	-1.60719300
C	-2.58129000	-1.11246500	0.17041000
H	-2.99940700	-0.10618800	0.24223800
C	1.26048500	1.35639800	2.45739600
O	-5.32331500	-0.86057100	0.44622100
C	4.92665800	-1.97802200	-0.45335500
C	2.81487100	3.16407100	1.62269500
H	3.14670400	3.39842000	2.63346600
C	3.33243100	3.85092200	0.54999900
H	4.07728100	4.63388800	0.70270600
C	-1.06012600	1.07399700	-4.71482800
H	-1.33499900	1.25011500	-5.75560900
C	-2.83431900	3.24485900	-1.37865500
H	-3.18748400	3.53991200	-2.36480500
C	0.03078300	-0.25796700	4.32493600
H	-0.45679900	-0.90176300	5.06313200
C	-2.86514100	3.46159000	0.97827900
H	-3.22665400	3.90872700	1.90355300
C	-3.33801000	3.85909800	-0.25582100
H	-4.09374100	4.64032600	-0.34511200
O	5.34991200	-0.81298900	-0.44811900
C	0.95128300	0.69071400	4.74379200
H	1.18990200	0.79956400	5.80329600
C	1.56587200	1.49566100	3.80842900
H	2.29379600	2.23870600	4.14471400
C	0.31977800	0.40537900	2.00155000
Na	-7.45360000	-1.70434600	0.64780800
Na	7.49096800	-1.62048000	-0.62624900

2-Na *C-trans-to-bpydc* E = –2264.290926; G = –2263.884569

Ru	0.00470500	0.45339000	0.02581000
N	-0.38354300	0.71715900	-1.95500600
O	-5.69782500	-3.03149500	0.28347200
N	1.22930600	-1.19413200	-0.15016700
O	5.52707500	-3.09525300	-0.65143900
N	-1.35194300	-1.19649700	0.07550000
N	-1.38606100	1.93582000	0.06024300
C	-1.28077000	1.66813600	-2.27393600
C	0.65417000	-2.41352700	-0.12775800
C	2.54984400	-1.12985400	-0.27437200
H	2.98403600	-0.12853900	-0.29337900
C	-2.93617700	-3.45766100	0.12434200
H	-3.56810500	-4.34665700	0.14543000
C	2.01012900	2.07143200	1.37463600
C	-0.79843800	-2.41504900	-0.00762900
C	-1.58983500	1.96320200	-3.59104900
H	-2.31235100	2.74343500	-3.82388600
C	0.20661800	0.05245300	-2.94413000
H	0.93250200	-0.70661400	-2.64524600

C	-1.57013700	-3.56659800	0.02030200
H	-1.10753600	-4.54983700	-0.04139500
C	-1.86637500	2.34486900	-1.12842100
C	2.77321400	-3.48670200	-0.36224000
H	3.38580300	-4.38492600	-0.44844200
C	3.36572300	-2.23665200	-0.38704700
C	-3.51077400	-2.20007400	0.20076200
C	1.99057400	2.59683300	-0.95248200
H	1.60567500	2.46523500	-1.97055300
C	-0.15558300	-0.31077400	2.94983400
H	-0.95485200	-0.95571500	2.57629500
C	-1.87148100	2.49724400	1.16344300
H	-1.45480900	2.13579200	2.10582300
C	-0.05351000	0.29206500	-4.27225100
H	0.46778900	-0.28765200	-5.03325900
C	1.40867100	-3.57104200	-0.23122400
H	0.92415200	-4.54532900	-0.21275000
C	-4.99215700	-2.01382500	0.29993100
C	3.01002500	3.51102000	-0.75387300
H	3.40348200	4.08158200	-1.60053700
C	-2.66814400	-1.10684900	0.17544600
H	-3.08261800	-0.09663300	0.24246400
C	1.43758600	1.27738700	2.44548100
O	-5.42197600	-0.85427200	0.38569300
C	4.84511600	-2.06724600	-0.54124800
C	3.03665400	2.99006000	1.57544000
H	3.45702700	3.15232900	2.57160300
C	3.53861500	3.71026700	0.51253800
H	4.34357500	4.43065200	0.66863100
C	-0.97081000	1.27020400	-4.60511700
H	-1.20065600	1.49316200	-5.64753400
C	-2.84528600	3.32002700	-1.21874600
H	-3.22330800	3.62989600	-2.19159000
C	0.17282100	-0.30680400	4.28498200
H	-0.36423600	-0.95561900	4.97552300
C	-2.84193100	3.47080000	1.14660800
H	-3.19722500	3.88905100	2.08765700
C	-3.34085900	3.89280500	-0.07059500
H	-4.11209400	4.66183300	-0.12573600
O	5.29519800	-0.91283600	-0.55472100
C	1.18832400	0.53080000	4.70665100
H	1.48485400	0.56470600	5.75643300
C	1.82094100	1.32469900	3.77944000
H	2.62263600	1.99396900	4.08897600
Na	-7.56449400	-1.69018600	0.39476200
Na	7.40156100	-1.77692700	-0.87023700
N	0.44837400	0.45158900	2.04522300
C	1.45637400	1.84139200	0.09486400

3-Et

Ru	0.06256500	0.50944900	-0.05379100
O	-5.80819400	-2.46579000	-0.01078700
N	-0.26756300	0.70245700	1.97197300
N	0.38857700	0.51987700	-2.06063000
N	-1.36602500	-0.98698500	-0.02573600
O	5.36332500	-3.51794700	0.30092800
N	1.61333200	1.81599500	-0.22593100
O	-5.40191500	-0.28365300	-0.15122200
C	2.10091000	2.01672700	-1.46430500
C	-0.90511700	-2.25625300	0.07225400
C	1.40687500	1.27907000	-2.50573100

C	-1.73338900	2.45253500	1.32594000
C	-1.79030100	2.85341800	-0.92634700
H	-1.42226800	2.56336800	-1.91487300
C	2.19223000	2.45571200	0.78572600
H	1.76904100	2.25897100	1.77259600
C	-1.15225800	1.63063600	2.38388900
C	3.17677400	2.85768200	-1.69226100
H	3.55569700	2.99961600	-2.70251400
C	0.53570500	-2.35609000	0.10724600
C	1.73484800	1.33545500	-3.84957700
H	2.56384200	1.95552900	-4.18506600
C	3.28999800	-2.39878400	0.17557600
C	1.21258700	-3.57100400	0.19904400
H	0.66748000	-4.51623000	0.24319400
C	-2.69178500	3.88247700	-0.78148600
H	-3.04626900	4.42328000	-1.65751100
C	3.26224700	3.30352400	0.63126500
H	3.69143400	3.79184000	1.50474100
C	-3.60644400	-1.79762500	-0.01854800
C	2.61695200	-1.18934100	0.08458400
H	3.21513800	-0.27518800	0.04479500
C	-0.29858800	-0.19145200	-2.94956300
H	-1.10695500	-0.80176500	-2.54316500
C	-1.46493300	1.78688500	3.72420800
H	-2.18613300	2.54055000	4.03319700
C	-1.79489500	-3.32339800	0.12566900
H	-1.41037000	-4.33843200	0.20502300
C	3.76962100	3.50947900	-0.63701300
H	4.61984500	4.17102100	-0.80174900
C	0.30625600	-0.06833100	2.89367100
H	1.01579200	-0.80500300	2.51252700
C	-2.64203600	3.47387800	1.55413800
H	-2.97443400	3.70768800	2.56341500
C	1.01379200	0.59973900	-4.76000900
H	1.26355400	0.63151700	-5.82030200
C	-2.67168900	-0.78443600	-0.06604300
H	-3.01666700	0.24957100	-0.14758700
C	-5.02870300	-1.41160700	-0.07118700
C	-0.02697500	-0.18103600	-4.29661600
H	-0.62857300	-0.78962300	-4.96984900
O	5.33823900	-1.30485100	0.13770800
C	-3.14804100	-3.10274000	0.08056400
H	-3.85694100	-3.92982200	0.12175300
C	-3.12976200	4.19620600	0.48991400
H	-3.84882000	4.99931600	0.65184300
C	0.04272200	0.03809600	4.23925900
H	0.54977000	-0.62564000	4.93792500
C	4.76657600	-2.49284300	0.21474000
C	-0.86541400	0.98512200	4.66680400
H	-1.10546800	1.09872800	5.72399800
C	2.58328600	-3.59381700	0.23420200
H	3.14041700	-4.52775100	0.30571400
C	-7.67847000	-2.00620500	-1.45793900
H	-7.43358400	-2.87722300	-2.07906900
H	-7.23325000	-1.11238900	-1.91131600
H	-8.76815000	-1.88074500	-1.47136100
C	-7.20389000	-2.19469100	-0.05338300
H	-7.41094400	-1.31092500	0.56760800
H	-7.66167200	-3.07320800	0.41935900
C	6.75531200	-1.32331800	0.16832900
H	7.04911900	-0.37563100	-0.30344000

H	7.11587800	-2.15356300	-0.45681800
C	7.27413200	-1.42924000	1.56696700
H	6.99856600	-2.38932900	2.01898300
H	6.88388800	-0.61878300	2.19668200
H	8.36913400	-1.35981700	1.56964300
N	-1.31827100	2.14603800	0.08999400
C	1.22638000	-1.12600300	0.05230700

3-Na E = –2264.292034

Ru	-0.00417700	0.43117900	0.00110500
N	-0.39790500	0.64001200	-1.98300500
O	-5.71496900	-3.00842800	0.36498700
N	1.24201900	-1.21145300	-0.14136200
O	5.53587200	-3.12583000	-0.60892000
N	1.54961000	1.89376600	0.13142900
N	-1.40792400	1.90382700	-0.00002600
C	-1.31296400	1.56549800	-2.32516900
C	0.65170500	-2.42516100	-0.07058000
C	2.55778400	-1.14772900	-0.28082200
H	2.99116100	-0.14670800	-0.34577900
C	-2.96191500	-3.37589400	0.21744800
H	-3.59818400	-4.25990700	0.27139000
C	2.04955200	2.10925400	1.35497600
C	-0.79058900	-2.36801200	0.04748100
C	-1.63693100	1.81059000	-3.64891000
H	-2.37836900	2.56647800	-3.90162900
C	0.19815900	-0.04608300	-2.95366500
H	0.93414900	-0.78649000	-2.63390800
C	-1.59599700	-3.50286600	0.11936900
H	-1.15686900	-4.50363300	0.09596100
C	-1.89950300	2.27096100	-1.19778600
C	2.77788300	-3.50266900	-0.27445500
H	3.39158600	-4.40359800	-0.32718400
C	3.37717100	-2.25559300	-0.35803300
C	-3.54122900	-2.11045000	0.24519900
C	2.04583800	2.58415700	-0.88539500
H	1.61028200	2.37147900	-1.86623600
C	-0.15306100	-0.26150400	2.93332900
H	-0.95229300	-0.91020000	2.57031700
C	-1.89669700	2.49230600	1.08750500
H	-1.47786300	2.16031300	2.03977000
C	-0.07401500	0.14727800	-4.28712800
H	0.45085400	-0.44901400	-5.03261600
C	1.41529000	-3.58418000	-0.13027400
H	0.92842400	-4.55657200	-0.06804500
C	-5.02909400	-1.97179000	0.34258600
C	3.05175100	3.51302200	-0.74877200
H	3.41776500	4.04886400	-1.62384300
C	-2.72961800	-0.98660700	0.17946300
H	-3.22210300	-0.00878000	0.21006200
C	1.43950200	1.30610100	2.41086600
O	-5.51014500	-0.82609500	0.39612900
C	4.84985700	-2.09545500	-0.53755200
C	3.06421000	3.02750100	1.57491800
H	3.46129500	3.19161500	2.57501000
C	3.57217800	3.73716900	0.51064800
H	4.37173500	4.46287800	0.66485200
C	-1.01310100	1.09535500	-4.64436400
H	-1.25752100	1.27708400	-5.69142300
C	-2.88773200	3.23394500	-1.31350000
H	-3.27215600	3.51176600	-2.29348000

C	0.17772200	-0.23184300	4.26762900
H	-0.36325700	-0.86800000	4.96722300
C	-2.87688100	3.45500600	1.04632500
H	-3.23514000	3.89496100	1.97627000
C	-3.38494600	3.83559300	-0.18099700
H	-4.16517400	4.59380600	-0.25549000
O	5.30242000	-0.94194000	-0.60613300
C	1.19310500	0.60620100	4.68127700
H	1.48963500	0.65765700	5.72941700
C	1.82680300	1.38179100	3.73853100
H	2.62959100	2.05249400	4.03841400
N	0.45225600	0.48232900	2.01091700
C	-1.33955100	-1.06580800	0.08514300
Na	-7.60249100	-1.73276300	0.51548700
Na	7.40852100	-1.81722800	-0.84944900

4-Na E = –2964.974478

Ru	-0.04495900	-0.92207000	-0.05398800
N	0.80368800	0.62818100	-1.25216000
N	-1.96384000	-0.76061600	-0.69386000
N	-0.78834900	0.48513700	1.20676200
N	0.50326900	-2.50158300	-1.27172100
N	1.91221200	-0.83986100	0.57548200
C	2.09293600	0.90736400	-1.01864200
C	-2.75062900	0.10982500	-0.03353100
C	-2.49224400	-1.44052800	-1.70839800
H	-1.82282000	-2.13678100	-2.21743500
C	-1.98887700	2.35452700	2.87466700
C	0.28693400	-3.74083400	-0.78562600
C	-2.08419100	0.81441500	1.04876700
C	2.75367600	1.91324000	-1.70174900
H	3.80169600	2.13724000	-1.50938100
C	0.15781100	1.34338400	-2.16317000
H	-0.89114100	1.07794700	-2.32456600
C	-2.70217500	1.74191200	1.86610100
H	-3.75174300	1.99761900	1.72792000
C	2.72159500	0.06917700	-0.00199000
C	-4.61654900	-0.40459200	-1.43699500
C	-3.79641100	-1.29399800	-2.11134500
C	-0.65484000	2.01254300	3.02428200
C	1.05794200	-2.36900500	-2.47095500
H	1.20420400	-1.34382000	-2.82039900
C	-1.20941600	-2.47561200	2.33810900
H	-1.44499100	-1.52003500	2.82096300
C	2.43370100	-1.63496600	1.50752400
H	1.74797200	-2.35694000	1.95405100
C	0.74517600	2.35801000	-2.88090100
H	0.16904400	2.91533400	-3.61855500
C	-4.07332100	0.30209700	-0.38491800
H	-4.69873000	1.00803500	0.15964000
C	1.42634100	-3.43623100	-3.25570600
H	1.87513600	-3.25940600	-4.23222400
C	-0.10269900	1.08414300	2.17727800
H	0.94374600	0.78928100	2.27678600
C	-0.33532200	-3.75821600	0.52518600
C	0.63987300	-4.86053200	-1.52693600
H	0.46012200	-5.85603600	-1.12308700
C	1.21209500	-4.71174200	-2.76814300
H	1.48989300	-5.58860200	-3.35561100
C	2.07717800	2.65443400	-2.64831000
C	4.04931800	0.19317700	0.36418900

H	4.68976200	0.93939100	-0.10303900
C	-1.51883800	-3.64318500	3.01334500
H	-1.99126300	-3.59416000	3.99888700
C	3.74383700	-1.56644100	1.91341200
H	4.10825000	-2.24343100	2.68512100
C	4.58066300	-0.62840900	1.33547800
C	-1.23363900	-4.87739600	2.44970100
H	-1.47552000	-5.79797100	2.98382500
C	-0.64336500	-4.93312600	1.20512200
H	-0.42424300	-5.90942200	0.76445400
C	-0.60172200	-2.48727200	1.08073600
C	2.77398200	3.75125200	-3.39986100
O	3.96959600	3.94995500	-3.14645600
O	2.10714400	4.38925600	-4.22634400
C	6.01595000	-0.49691800	1.75292500
O	6.44381100	-1.31203500	2.58137100
O	6.68103100	0.41414900	1.24017100
C	-2.64366300	3.35752300	3.77632200
O	-3.84717500	3.58665000	3.58956700
O	-1.94221100	3.89596400	4.64369300
C	-6.05082300	-0.21183800	-1.82849400
O	-6.47800500	-0.87442200	-2.78371000
O	-6.72101100	0.59195800	-1.16458400
H	-0.04516700	2.46864400	3.80337500
H	-4.17483700	-1.87746500	-2.94987000
Na	8.48250000	-0.27095100	2.47030900
Na	3.95858700	5.64354000	-4.70121900
Na	-3.76901400	5.08031700	5.33106100
Na	-8.52545200	0.14108900	-2.47573800

1-H E = –1957.296484

Ru	0.00938300	-0.31284400	0.00169200
N	-0.71955800	-0.43180600	1.91566000
O	-5.53324100	3.05905200	-1.01298200
N	1.23744200	1.30572300	0.26701100
O	5.49067300	3.20009500	1.05105000
N	-1.27695000	1.25766100	-0.27424900
N	1.44235700	-1.76730700	0.16886200
N	-1.36903000	-1.81975800	-0.15692800
N	0.73600000	-0.42001800	-1.91218500
C	-1.68282100	-1.34224400	2.13135500
C	0.67199400	2.51934500	0.13297500
C	2.53386200	1.23313500	0.52297100
H	2.95104000	0.23062700	0.63337900
C	-2.88480100	3.49812100	-0.51077300
H	-3.51831800	4.38033700	-0.59770000
C	2.11142000	-2.07788800	-0.95403300
C	-0.75765500	2.49239500	-0.13632900
C	-2.26583200	-1.49471500	3.37687000
H	-3.04691900	-2.23661500	3.53205200
C	-0.32537400	0.33252500	2.92632400
H	0.46508800	1.05317500	2.70645300
C	-1.54261200	3.62639500	-0.24563500
H	-1.10661700	4.61511200	-0.11967200
C	-2.03804000	-2.13862300	0.96366700
C	2.75774700	3.60134100	0.50687500
H	3.37067600	4.49842800	0.60003700
C	3.33275400	2.35222600	0.65346600
C	-3.40893800	2.22712500	-0.66660700
C	1.73489900	-2.41936800	1.28706700
H	1.17152300	-2.13004700	2.17654500

C	0.31288700	0.32343600	-2.92680100
H	-0.49700700	1.02261500	-2.70832400
C	-1.63282800	-2.49196700	-1.27035200
H	-1.07057700	-2.19613400	-2.15845600
C	-0.85943500	0.23418700	4.19033200
H	-0.49294700	0.88883600	4.97977500
C	1.41297400	3.68300800	0.24478400
H	0.93913100	4.65459400	0.12276700
C	-4.82941800	1.96082300	-0.96145000
C	2.69577300	-3.40204600	1.34942900
H	2.89141900	-3.90088700	2.29758400
C	-2.56678200	1.14113300	-0.53718700
H	-2.96032400	0.12884400	-0.65428400
C	1.72489900	-1.30314400	-2.12632200
O	-5.27474300	0.86518900	-1.13084700
C	4.77625400	2.25018700	0.93913300
C	3.08861600	-3.05699600	-0.96422300
H	3.61882600	-3.29657000	-1.88383400
C	3.38540100	-3.72814000	0.20004200
H	4.15327600	-4.50256800	0.20819700
C	-1.85082800	-0.69775400	4.41931300
H	-2.30074400	-0.80576200	5.40673700
C	-2.98781300	-3.14432000	0.97576600
H	-3.51980600	-3.38847100	1.89315500
C	0.84156900	0.22911100	-4.19339400
H	0.45088000	0.86536800	-4.98627900
C	-2.56546500	-3.50158800	-1.33062000
H	-2.73889100	-4.01503500	-2.27526800
C	-3.25616700	-3.83484900	-0.18405600
H	-4.00312000	-4.62945100	-0.19099000
O	5.17395200	1.01098200	1.05362200
C	1.85908900	-0.67467400	-4.42072100
H	2.30560300	-0.77810200	-5.41016200
C	2.30470300	-1.44914500	-3.37401100
H	3.10750700	-2.16789900	-3.52761300
H	6.11835100	1.01467100	1.23475000
H	-6.44604500	2.82384300	-1.20437400

2-H E = –1940.772245

Ru	0.02676100	-0.28914100	-0.01092400
N	-0.65073900	-0.47992800	2.01384500
O	-5.50494300	3.09400500	-0.97878100
N	1.25684400	1.30839700	0.23549300
O	5.51787200	3.16886100	1.07748800
N	-1.24997400	1.27444300	-0.24535100
N	1.47265800	-1.76160600	0.07564400
N	-1.37634300	-1.79833400	-0.10080800
C	-1.61306200	-1.38612200	2.22412600
C	0.69621300	2.53192500	0.14635700
C	2.55976700	1.22930200	0.47128700
H	2.97596200	0.22247400	0.53493600
C	-2.85494300	3.52778100	-0.48880400
H	-3.48577700	4.41110000	-0.58078200
C	2.06573900	-2.09437100	-1.08960000
C	-0.72958900	2.51306500	-0.11518600
C	-2.18050100	-1.56744300	3.47552100
H	-2.96831100	-2.30241300	3.62994300
C	-0.23443200	0.25185400	3.03711000
H	0.55883500	0.97315500	2.81977200

C	-1.51274900	3.64980700	-0.22901600
H	-1.06975300	4.63700500	-0.11348100
C	-2.00128300	-2.14701900	1.03963200
C	2.78717400	3.59884200	0.54817500
H	3.40229700	4.49020600	0.67307100
C	3.36041600	2.34061900	0.63747600
C	-3.38272900	2.25392700	-0.63419200
C	1.83396900	-2.39608000	1.18496700
H	1.32742100	-2.08330600	2.10147300
C	0.13677300	0.39327700	-3.00917500
H	-0.64210600	1.14745000	-2.84666600
C	-1.69491000	-2.45324300	-1.21404000
H	-1.16950900	-2.13911900	-2.11757900
C	-0.74513400	0.12997900	4.30942500
H	-0.36166400	0.76110800	5.11040600
C	1.44233100	3.68979500	0.29778600
H	0.96724500	4.66533100	0.21739400
C	-4.80376700	1.99228900	-0.92076800
C	2.78946800	-3.38451200	1.21286900
H	3.04194900	-3.86506700	2.15709800
C	-2.54459900	1.16670400	-0.50381300
H	-2.94182500	0.15537700	-0.61687700
C	1.60238800	-1.32012800	-2.22582100
O	-5.26059400	0.89892100	-1.07960700
C	4.80491300	2.22593900	0.90277100
C	3.03395900	-3.08867400	-1.12979400
H	3.50360500	-3.34928300	-2.07751400
C	3.40042600	-3.73881500	0.02478400
H	4.16223000	-4.52003900	-0.00033700
C	-1.74139100	-0.80016400	4.53048300
H	-2.17757300	-0.92821500	5.52201500
C	-2.94900900	-3.15631100	1.06754100
H	-3.43768700	-3.42421800	2.00214400
C	0.62469300	0.22219700	-4.29283200
H	0.23639200	0.83683100	-5.11040600
C	-2.63083000	-3.46004700	-1.25804500
H	-2.84396200	-3.95059700	-2.20709200
C	-3.27194600	-3.82242300	-0.09159800
H	-4.01802900	-4.61789600	-0.08213800
O	5.21520900	0.98460200	0.92456600
C	1.60419600	-0.72447600	-4.55137300
H	1.98833300	-0.85949600	-5.56399400
C	2.09187100	-1.49445200	-3.51705900
H	2.86602800	-2.23718500	-3.72704400
H	6.16174700	0.98686600	1.09423900
H	-6.41857800	2.85822300	-1.16465800
C	0.59954100	-0.36935000	-1.93492200

3-H E = –1940.779000

Ru	0.00252000	-0.30797400	0.01236000
N	-0.63685400	-0.54917800	1.93253300
O	-5.64872900	3.07252600	-0.87412600
N	1.18784200	1.35809800	0.30838100
O	5.40102100	3.33374800	1.13452700
N	1.56377600	-1.77288800	0.05525300
N	-1.34458700	-1.82315300	-0.17549500
C	-1.54470100	-1.51764800	2.14886700
C	0.58128100	2.56263300	0.20173900
C	2.48661500	1.31537500	0.55436900
H	2.92631700	0.31928500	0.64058600
C	-3.00368400	3.45069100	-0.41134900

H	-3.64673000	4.32643300	-0.49011200
C	2.17236700	-2.00974600	-1.11368200
C	-0.83952900	2.47689800	-0.05762200
C	-2.02695300	-1.79004500	3.41777900
H	-2.75872200	-2.58208700	3.56760000
C	-0.21069500	0.15993100	2.97273600
H	0.52089600	0.94010400	2.75317100
C	-1.66040700	3.59812900	-0.16371300
H	-1.25422300	4.60544400	-0.04752500
C	-1.95288300	-2.23457100	0.95152900
C	2.65290200	3.68640400	0.59484200
H	3.24456400	4.59623200	0.70717200
C	3.26438900	2.44712400	0.70838300
C	-3.53126600	2.16967700	-0.55784300
C	1.92992800	-2.48028800	1.11435700
H	1.41040200	-2.24855600	2.04880800
C	0.24235000	0.45331200	-2.89570600
H	-0.57216200	1.12413800	-2.61719400
C	-1.66991200	-2.41703500	-1.31948000
H	-1.15943500	-2.05048500	-2.21248100
C	-0.64612400	-0.05685900	4.25863400
H	-0.25547700	0.55984900	5.06725700
C	1.30775500	3.73889600	0.34054200
H	0.80779900	4.70105100	0.24410900
C	-4.96307800	1.95309600	-0.82092600
C	2.90570500	-3.45019500	1.07424400
H	3.16273400	-3.99846200	1.97996700
C	-2.71000600	1.05698800	-0.45257500
H	-3.17511100	0.07360500	-0.57892700
C	1.70914300	-1.17778500	-2.22087000
O	-5.47078900	0.87735900	-0.97176900
C	4.70415000	2.37319700	0.98098500
C	3.16247000	-2.97150900	-1.23670200
H	3.64450600	-3.15756100	-2.19472000
C	3.53377400	-3.70028000	-0.12966000
H	4.31096600	-4.46165000	-0.20818600
C	-1.57358600	-1.05434400	4.48793600
H	-1.94255900	-1.25692400	5.49390700
C	-2.89600700	-3.24786600	0.93995600
H	-3.37641900	-3.56110400	1.86519500
C	0.73133700	0.43639900	-4.18089200
H	0.30135100	1.10502300	-4.92572100
C	-2.59881500	-3.42693700	-1.40428700
H	-2.82224300	-3.86925700	-2.37442800
C	-3.22653500	-3.85308400	-0.25012900
H	-3.97024500	-4.65020300	-0.27696500
O	5.14615800	1.14081800	1.03678800
C	1.75884000	-0.43162000	-4.48864900
H	2.17652900	-0.47602100	-5.49503400
C	2.25007200	-1.24458200	-3.49399600
H	3.06363100	-1.93452000	-3.70894400
H	6.09120400	1.17387900	1.20954400
H	-6.56653800	2.84355800	-1.04507100
N	0.70531400	-0.33059800	-1.92566000
C	-1.34250300	1.16189400	-0.20119800

4-H E = –2317.935864

Ru	0.03981600	-0.61463300	0.04012900
N	-0.85302900	0.92305700	1.21371000
N	1.93130900	-0.45636700	0.73880000
N	0.82272500	0.78076700	-1.20197400

N	-0.53797600	-2.19839400	1.24469900
N	-1.89476600	-0.54631800	-0.64890500
C	-2.13700200	1.19373600	0.94378800
C	2.74836400	0.39446100	0.08968200
C	2.41513400	-1.12621400	1.78266100
H	1.72169600	-1.80359000	2.28293200
C	2.07757000	2.60706800	-2.85816800
C	-0.30452800	-3.43549400	0.76354900
C	2.11990900	1.09390100	-1.01721600
C	-2.82014500	2.19681800	1.60579700
H	-3.86159500	2.42552900	1.38493000
C	-0.23448800	1.63282500	2.14680800
H	0.80909800	1.36959300	2.33887400
C	2.76767800	2.00304400	-1.82911300
H	3.81705600	2.25149200	-1.67628900
C	-2.73006100	0.34997300	-0.08871700
C	4.55400800	-0.12364700	1.55562900
C	3.70591000	-0.99040500	2.22376100
C	0.74187300	2.28645900	-3.04058000
C	-1.12118200	-2.06659200	2.43018900
H	-1.27810100	-1.04259500	2.77794600
C	1.26989900	-2.16547100	-2.32040700
H	1.51395000	-1.21018700	-2.79873900
C	-2.37583700	-1.34149500	-1.60300400
H	-1.66913700	-2.05094000	-2.03514900
C	-0.84181800	2.64456600	2.85166800
H	-0.28174800	3.19374200	3.60624100
C	4.06291900	0.57773200	0.47413800
H	4.70483100	1.26758500	-0.06975500
C	-1.50599200	-3.13560700	3.20418600
H	-1.97861400	-2.96103200	4.16965500
C	0.16317200	1.37643500	-2.19215900
H	-0.88479600	1.09638000	-2.30964000
C	0.35329200	-3.45071000	-0.52970900
C	-0.67360400	-4.55675200	1.49390900
H	-0.48130000	-5.55117100	1.09343100
C	-1.27728000	-4.40969000	2.72014700
H	-1.56795500	-5.28752800	3.29977300
C	-2.16609100	2.93376500	2.57010800
C	-4.05227700	0.45474300	-0.47907100
H	-4.71032300	1.18386200	-0.01169900
C	1.60127600	-3.33290200	-2.98600200
H	2.09893100	-3.28226500	-3.95869400
C	-3.67442000	-1.28991700	-2.04283200
H	-4.01316000	-1.96293500	-2.82936100
C	-4.53613600	-0.37325900	-1.46981300
C	1.30662600	-4.56690000	-2.42834200
H	1.56621600	-5.48690600	-2.95491700
C	0.68366400	-4.62457300	-1.20004900
H	0.45652900	-5.60076400	-0.76391700
C	0.63193200	-2.18197600	-1.07991100
C	-2.91470000	4.00742000	3.25833200
O	-4.06014600	4.26220800	3.03507900
O	-2.17536100	4.63994100	4.12957900
H	-2.71013000	5.32684900	4.53821400
C	-5.93515600	-0.31502000	-1.94107600
O	-6.36550200	-1.01558800	-2.80762400
O	-6.63716300	0.58486200	-1.30531700
H	-7.53175700	0.57237100	-1.65823300
C	2.79769800	3.56524200	-3.71962900
O	3.94552700	3.86087500	-3.56594600

O	2.03605700	4.04613000	-4.66616400
H	2.56175700	4.65564900	-5.19215500
C	5.94493400	0.01550800	2.02842100
O	6.38384100	-0.58321500	2.96496300
O	6.63416300	0.86215900	1.30979000
H	7.52438500	0.90630100	1.67115400
H	0.14800200	2.73458000	-3.83510500
H	4.05427300	-1.56077900	3.08375900

References

1. A. Spek, *Acta Crystallogr. Sect. C*, **2015**, 71, 9-18.
2. Gaussian 09, Revision D.01, Frisch et al., Gaussian, Inc., Wallingford CT, 2013.
3. Peverati, R.; Truhlar, D. G.; *J. Phys. Chem. Lett.*, **2012**, *3*, 117.
4. Scalmani, G.; Frisch, M. J.; Mennucci, B.; Tomasi, J.; Cammi, R.; Barone, V.; *J. Chem. Phys.*, **2006**, *124*, 094107.
5. (a) Gorelsky, S. I. *AOMix: Program for Molecular Orbital Analysis*; version 6.85, University of Ottawa, 2013, http://www.sg-chem.net/; (b) Gorelsky, Si. I.; Lever, A. B. P.; *J. Organomet. Chem.*, **2001**, *635*, 187.
6. Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A.; *J. Chem. Phys.*, **1980**, *72*, 650.
7. Roy, L. E.; Hay, P. J.; Martin, R. L.; *J. Chem. Theory Comput.*, **2008**, *4*, 1029.
8. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G.; *J. Phys. Chem. B*, **2009**, *113*, 6378.
9. Perdew, J. P.; Burke, K.; Ernzerhof, M.; *Phys. Rev. Lett.*, **1996**, *77*, 3865.
10. Vydrov, O. A.; Scuseria, G. E.; *J. Chem. Phys.*, **2006**, *125*, 234109.
11. Peverati, R.; Truhlar, D. G.; *J. Phys. Chem. Lett.*, **2011**, *2*, 2810.
12. Adamo, C.; Barone, V.; *J. Chem. Phys.*, **1999**, *110*, 6158.
13. Zhao, Y.; Truhlar, D. G.; *Theor. Chem. Acc.*, **2008**, *120*, 215.
14. Becke, A. D.; *J. Chem. Phys.*, **1993**, *98*, 5648.
15. Yanai, T.; Tew, D.; Handy, N.; *Chem. Phys. Lett.*, **2004**, *393*, 51.
16. Chai, J.-D.; Head-Gordon, M.; *Phys. Chem. Chem. Phys.*, **2008**, *10*, 6615.
17. Nazeeruddin, M. K.; De Angelis, F.; Fantacci, S.; Selloni, A.; Viscardi, G.; Liska, P.; Ito, S.; Takeru, B.; Grätzel, M.; *J. Am. Chem. Soc.*, **2005**, *127*, 16835.
18. Kupfer, S.; Wächtler, M. S.; Guthmuller, J.; Popp, J.; Dietzek, B.; González, L.; *J. Phys. Chem. C*, **2012**, *116*, 19968.