A new model for mapping the peptide backbone: predicting proton chemical shifts in proteins

(Supporting Information)

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- **Table S1.** Deshieldings (ppm) on N–C(=O)–CH protons for **1-15** in $CDCl_3$.
- **Figures S1 and S2.** Linear relationships between σ'_H and the function $\cos^2[(\psi-10)/2]/d'$ in DMSO-d_6 and D_2O for amides **1-15**.
- **Table S2.** Experimental and calculated chemical shifts from dimeric insulin alpha protons.
- Minimum energy structures for *Z*-amides **1-15** obtained by B3PW91/6-31G* calculations.
- ^{1}H-NMR spectra from amides **1-15** in $CDCl_3$, DMSO-d_6 and D_2O.

Table S1. Deshieldings (ppm) on N–C(=O)–CH protons for **1-15** in $CDCl_3$

Compound	δ_{obs}	x, y	σ'_{amide}	σ'_{anti}	σ'_{gauche}	$\sigma'_{anti} - \sigma'_{gauche}$
1	1.99	(H, H)	1.08	0.76	1.24	-0.48
2	1.97	(H, H)	1.06	0.76	1.21	-0.45
3	1.95	(H, H)	1.04	0.76	1.18	-0.42
4	2.02	(H, H)	1.11	0.76	1.29	-0.53
5	2.03	(H, H)	1.12	0.76	1.30	-0.54
6	2.07	(H, H)	1.16	0.76	1.36	-0.60
7	2.22	(H, Me)	0.97	0.76	1.18	-0.42
8	2.19	(H, Me)	0.94	0.76	1.12	-0.36
9	2.16	(H, Me)	0.91	0.76	1.06	-0.30
10	2.36	(Me, Me)	0.77	0.77*		
11	2.33	(Me, Me)	0.74	0.74*		
12	2.29	(Me, Me)	0.70	0.70*		
13	3.55	(Me, Ph)	0.81	0.81*		
14	3.53	(Me, Ph)	0.79	0.79*		
15	3.50	(Me, Ph)	0.76	0.76*		
Average ± SD				0.76 ± 0.02	1.22 ± 0.09	-0.46 ± 0.09

* σ'_{anti} values whose average has been taken as σ'_{anti} for amides with more than one proton on CH (n>1, **1**-**9**).

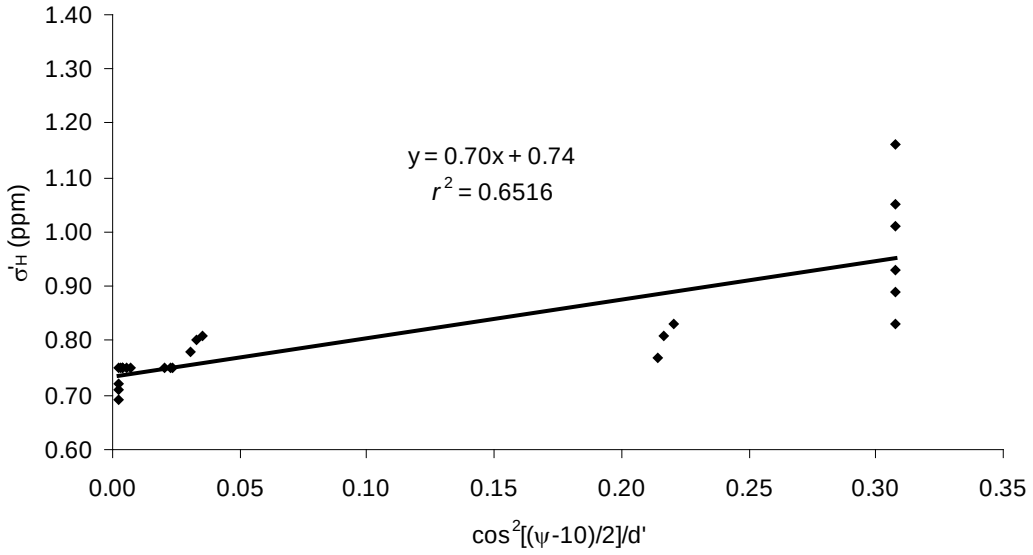


Figure S1. Linear relationship between σ'_H and the function $\cos^2[(\psi\text{-}10)/2]/d'$ in DMSO-d_6 for amides **1-15**

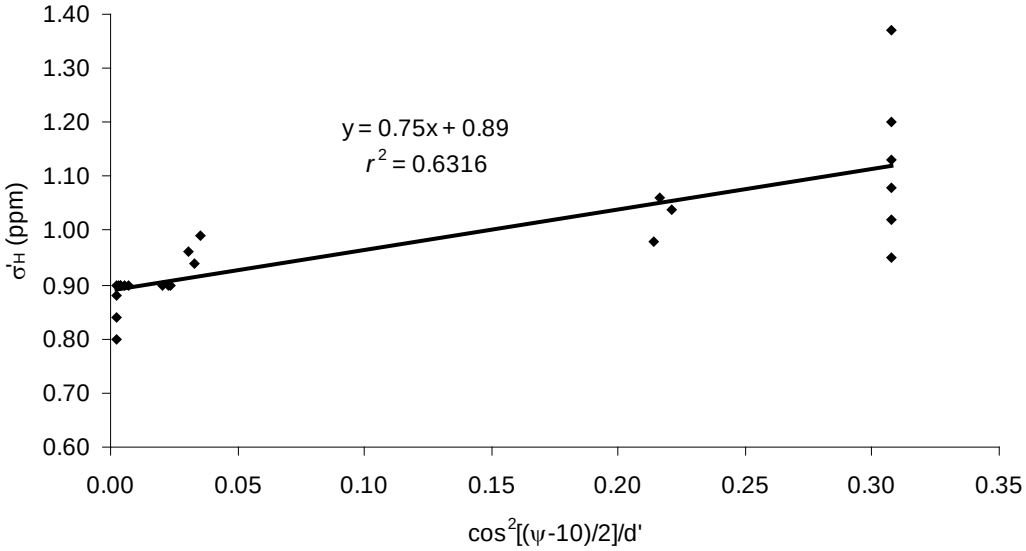


Figure S2. Linear relationship between σ'_H and the function $\cos^2[(\psi\text{-}10)/2]/d'$ in D_2O for amides **1-15**

Table S2. Experimental and calculated chemical shifts from dimeric insulin alpha protons

#	Amino acid	δ_{obs} (ppm)	α (º)	d (Å)	ψ (º)	d' (Å)	σ_R (ppm)	δ_{calc} (ppm)	$\delta_{calc} - \delta_{obs}$ (ppm)
1	GLY								
1	GLY								
2	ILE	3.78	51.3	2.73	20.0	2.35	0.65	4.22	-0.44
3	VAL	3.53	58.5	2.75	18.7	2.48	0.72	4.22	-0.69
4	GLU	4.09	45.3	2.62	17.5	2.60	0.77	4.37	-0.28
5	GLN	4.01	66.3	2.87	13.4	2.68	0.70	4.11	-0.10
6	CYS	4.82	61.6	2.85	17.2	2.64	1.22	4.67	0.15
7	CYS	4.79	31.4	2.61	9.4	2.35	1.22	4.91	-0.12
8	THR	4.02	43.8	2.57	29.3	2.57	0.93	4.54	-0.52
9	SER	4.66	6.8	2.31	59.5	2.88	1.05	4.65	0.01
10	ILE	4.45	24.4	2.44	140.5	3.20	0.65	4.10	0.35
11	CYS	5.07	34.2	2.45	130.8	3.13	1.22	4.67	0.40
12	SER	4.57	1.9	2.61	149.3	3.12	1.05	4.38	0.19
13	LEU	3.94	45.3	2.85	27.6	2.39	0.90	4.48	-0.54
14	TYR	4.14	50.9	2.74	18.4	2.55	1.21	4.76	-0.62
15	GLN	3.96	34.9	2.77	20.1	2.38	0.70	4.34	-0.38
16	LEU	4.11	54.1	2.70	31.2	2.64	0.90	4.42	-0.31
17	GLU	4.13	55.8	2.71	39.2	2.58	0.77	4.27	-0.14
18	ASN	4.41	44.6	2.42	53.6	2.63	1.18	4.78	-0.37
19	TYR	4.40	34.7	2.60	56.3	2.77	1.21	4.80	-0.40
20	CYS	4.72	42.1	2.34	134.9	3.17	1.22	4.66	0.06
21	ASN	4.52	44.6	2.51	153.5	3.22	1.18	4.54	-0.02
1	PHE								
2	VAL	4.08	0.3	2.47	138.7	3.27	0.72	4.07	0.01
3	ASN	4.62	33.2	2.58	145.3	3.21	1.18	4.58	0.04
4	GLN	4.36	0.0	2.24	150.1	3.29	0.70	4.08	0.28

#	Amino acid	δ_{obs} (ppm)	α (º)	d (Å)	ψ (º)	d' (Å)	σ_R (ppm)	δ_{calc} (ppm)	$\delta_{calc} - \delta_{obs}$ (ppm)
5	HIS	4.42	1.1	2.13	170.9	3.27	1.09	4.48	-0.06
6	LEU	4.44	0.3	2.43	171.3	3.22	0.90	4.22	0.22
7	CYS	4.86	10.5	2.51	142.6	3.09	1.22	4.62	0.24
8	GLY	3.93	163.5	3.81	59.5	2.86	0.59	3.87	0.06
8	GLY	3.74	71.7	3.06	168.4	3.31	0.59	3.67	0.07
9	SER	4.04	67.2	2.60	52.3	2.79	1.05	4.43	-0.39
10	HIS	4.49	44.9	2.48	36.5	2.52	1.09	4.71	-0.22
11	LEU	3.97	40.7	2.64	21.7	2.37	0.90	4.55	-0.58
12	VAL	3.37	59.8	2.75	27.8	2.71	0.72	4.18	-0.81
13	GLU	4.02	47.7	2.74	12.9	2.55	0.77	4.34	-0.32
14	ALA	4.03	49.0	2.80	17.5	2.42	0.75	4.32	-0.29
15	LEU	3.90	44.6	2.79	21.4	2.45	0.90	4.49	-0.59
16	TYR	4.16	47.7	2.86	10.6	2.51	1.21	4.77	-0.61
17	LEU	4.02	52.1	2.68	14.1	2.61	0.90	4.45	-0.43
18	VAL	3.80	65.8	2.98	5.7	2.66	0.72	4.12	-0.32
19	CYS	4.70	32.9	2.51	30.5	2.64	1.22	4.88	-0.18
20	GLY	3.85	177.4	3.62	80.0	2.90	0.59	3.92	-0.07
20	GLY	3.85	61.0	2.62	1.0	3.25	0.59	4.02	-0.17
21	GLU	4.20	60.0	2.77	55.2	2.76	0.77	4.19	0.01
22	ARG	4.16	40.8	2.55	35.4	2.51	0.80	4.43	-0.27
23	GLY	3.77	167.2	3.87	130.3	3.07	0.59	3.73	0.04
23	GLY	3.87	31.0	2.74	116.4	3.12	0.59	4.02	-0.15
24	PHE	4.64	32.3	2.48	123.8	3.10	1.26	4.73	-0.09
25	PHE	4.56	8.0	2.59	163.8	3.18	1.26	4.61	-0.05
26	TYR	4.56	0.9	2.45	170.0	3.27	1.21	4.54	0.02
27	THR	4.54	1.0	2.23	145.6	3.26	0.93	4.33	0.21
28	PRO	4.31	38.4	2.65	140.3	3.07	1.01	4.39	-0.08
29	LYS	4.33	28.0	2.43	153.5	3.20	0.82	4.25	0.08
30	ALA	4.20	64.4	2.94	163.0	3.24	0.75	3.90	0.30
1	GLY								
1	GLY								
2	ILE	3.78	59.0	2.91	22.1	2.52	0.65	4.13	-0.35
3	VAL	3.53	45.4	2.60	17.7	2.49	0.72	4.33	-0.80
4	GLU	4.09	62.0	3.05	4.4	2.65	0.77	4.20	-0.11
5	GLN	4.01	49.0	2.65	23.5	2.57	0.70	4.27	-0.26
6	CYS	4.82	11.9	2.13	44.1	2.61	1.22	4.94	-0.12
7	CYS	4.79	29.8	2.46	3.2	2.73	1.22	4.90	-0.11
8	THR	4.02	41.5	2.71	6.9	2.48	0.93	4.55	-0.53
9	SER	4.66	27.9	2.29	82.8	2.90	1.05	4.66	0.00
10	ILE	4.45	18.6	2.50	149.3	3.20	0.65	4.07	0.38
11	CYS	5.07	24.9	2.74	149.7	3.10	1.22	4.60	0.47
12	SER	4.57	24.2	2.65	141.0	3.13	1.05	4.46	0.11
13	LEU	3.94	47.0	2.58	37.8	2.57	0.90	4.49	-0.55
14	TYR	4.14	47.4	2.80	20.0	2.48	1.21	4.78	-0.64
15	GLN	3.96	46.0	2.61	25.6	2.59	0.70	4.29	-0.33
16	LEU	4.11	56.7	2.63	35.4	2.65	0.90	4.40	-0.29
17	GLU	4.13	53.4	2.66	49.7	2.70	0.77	4.27	-0.14
18	ASN	4.41	48.2	2.72	37.0	2.64	1.18	4.73	-0.32
19	TYR	4.40	17.6	2.55	59.5	2.53	1.21	4.83	-0.43
20	CYS	4.72	41.9	2.79	154.9	3.23	1.22	4.54	0.18
21	ASN	4.52	33.0	2.70	130.6	3.18	1.18	4.59	-0.07

#	Amino acid	δ_{obs} (ppm)	α (º)	*d* (Å)	ψ (º)	*d'* (Å)	σ_R (ppm)	δ_{calc} (ppm)	$\delta_{calc} - \delta_{obs}$ (ppm)
1	PHE								
2	VAL	4.08	6.9	2.08	126.7	3.14	0.72	4.23	-0.15
3	ASN	4.62	33.9	2.65	170.8	3.32	1.18	4.54	0.08
4	GLN	4.36	14.4	2.32	148.9	3.26	0.70	4.15	0.21
5	HIS	4.42	24.0	2.32	178.1	3.22	1.09	4.53	-0.11
6	LEU	4.44	1.9	2.34	173.0	3.34	0.90	4.25	0.19
7	CYS	4.86	3.8	2.51	161.2	3.21	1.22	4.56	0.30
8	GLY	3.74	166.3	3.78	73.5	2.97	0.59	3.85	-0.11
8	GLY	3.93	47.8	2.82	173.4	3.18	0.59	3.86	0.07
9	SER	4.04	53.9	2.66	34.6	2.60	1.05	4.57	-0.53
10	HIS	4.49	56.2	2.68	30.0	2.63	1.09	4.60	-0.11
11	LEU	3.97	31.1	2.55	19.3	2.20	0.90	4.62	-0.65
12	VAL	3.37	48.0	2.44	38.5	2.53	0.72	4.33	-0.96
13	GLU	4.02	42.7	2.65	26.0	2.57	0.77	4.38	-0.36
14	ALA	4.03	41.7	2.44	30.6	2.53	0.75	4.40	-0.37
15	LEU	3.90	59.8	2.74	16.4	2.70	0.90	4.37	-0.47
16	TYR	4.16	57.7	2.76	15.0	2.60	1.21	4.71	-0.55
17	LEU	4.02	53.3	2.80	16.9	2.47	0.90	4.44	-0.42
18	VAL	3.80	54.8	3.08	0.5	2.59	0.72	4.20	-0.40
19	CYS	4.70	26.5	2.61	15.1	2.25	1.22	4.93	-0.23
20	GLY	3.85	160.9	3.90	56.4	2.75	0.59	3.86	-0.01
20	GLY	3.85	73.3	3.15	169.4	3.38	0.59	3.65	0.20
21	GLU	4.20	54.7	2.61	45.7	2.62	0.77	4.28	-0.08
22	ARG	4.16	45.0	2.91	18.2	2.52	0.80	4.37	-0.21
23	GLY	3.77	156.6	3.74	140.7	2.99	0.59	3.66	0.11
23	GLY	3.87	22.6	2.35	109.4	2.94	0.59	4.13	-0.26
24	PHE	4.64	33.3	2.69	131.9	3.10	1.26	4.67	-0.03
25	PHE	4.56	11.8	2.63	166.8	3.22	1.26	4.61	-0.05
26	TYR	4.56	3.1	2.64	159.5	3.22	1.21	4.53	0.03
27	THR	4.54	5.8	2.40	149.5	3.19	0.93	4.32	0.22
28	PRO	4.31	14.5	2.80	25.1	1.36	1.01	4.88	-0.57
29	LYS	4.33	45.9	2.73	45.3	2.59	0.82	4.37	-0.04
30	ALA	4.20	51.3	2.56	150.2	3.29	0.75	4.06	0.14

* Calculation of chemical shifts from amino-terminus residues is not possible, since α dihedral angle and *d* distance require a previous residue.

Minimum energy structures for *Z*-amides **1**-**15** obtained by B3PW91/6-31G* calculations

B3PW91/6-31G* Structure 1 Z
Energy: -248.430841
# of imaginary frequencies = 0

C	-0.002395	-0.000009	0.006502
C	-0.003424	0.000114	1.524424
O	1.035931	-0.000078	2.168937
N	-1.239303	-0.000066	2.104872
C	-1.422287	-0.000136	3.537764
H	-2.054502	0.000052	1.511723
H	0.543644	-0.881026	-0.344089
H	-1.000790	0.000067	-0.442970
H	0.543848	0.880832	-0.344207
H	-1.966524	-0.891753	3.872066
H	-0.427511	-0.000536	3.987208
H	-1.965867	0.891808	3.872281

B3PW91/6-31G* Structure 2 Z
Energy: -287.733734
# of imaginary frequencies = 0

C	-0.016945	-0.055918	-0.008903
C	0.014805	0.045141	1.513744
N	1.359456	0.037487	2.057119
C	1.964632	1.163047	2.538513
C	3.395595	0.978655	3.011302
O	1.402234	2.247679	2.598647
H	1.900420	-0.811329	1.986227
H	-0.434428	0.984926	1.844784
H	-0.556845	-0.776476	1.964566
H	-1.051081	-0.049715	-0.371986
H	0.510907	0.789794	-0.461181
H	0.454580	-0.981629	-0.360863
H	4.046203	1.638895	2.429544
H	3.766607	-0.048034	2.927980
H	3.462715	1.295853	4.056208

B3PW91/6-31G* Structure 3 Z
Energy: -327.036271
# of imaginary frequencies = 0

C	-0.057725	-0.031197	0.052317
C	0.043289	0.018384	1.575704
C	1.494739	0.030718	2.060740
N	-0.695007	1.164233	2.090084
C	-1.532276	1.084885	3.164288
O	-1.759175	0.037730	3.755772
C	-2.177785	2.394450	3.583123
H	-0.462549	-0.852155	2.004968
H	-0.513383	2.068755	1.679243
H	-3.261251	2.251369	3.626801
H	-1.842394	2.646058	4.594342
H	-1.955980	3.235156	2.917799
H	-1.103093	-0.072538	-0.270338
H	0.459076	-0.914175	-0.339099
H	0.408327	0.851788	-0.405495
H	2.029242	0.913917	1.687788
H	2.029974	-0.858597	1.708296
H	1.531885	0.042268	3.154449

B3PW91/6-31G* Structure 4 Z
Energy: -518.695316
# of imaginary frequencies = 0

C	-0.011844	0.055593	-0.000999
C	-0.005741	0.046607	1.395085
C	1.197228	-0.007638	2.103230
C	2.398330	-0.049368	1.381449
C	2.394706	-0.039638	-0.009620
C	1.186746	0.011860	-0.707229
C	1.265573	-0.054272	3.625430
N	1.649451	-1.387938	4.081955
C	2.906447	-1.683912	4.522521
O	3.791154	-0.843467	4.629859
C	-0.000742	0.402616	4.345561
C	3.141322	-3.138538	4.885270
H	2.243913	-3.762754	4.829427
H	3.902070	-3.550926	4.214720
H	3.544379	-3.184150	5.900987
H	1.004401	-2.145386	3.906824
H	2.098905	0.581256	3.942761
H	-0.292722	1.406952	4.021207
H	-0.845981	-0.271421	4.159651
H	0.176490	0.424296	5.424947
H	3.339115	-0.088341	1.926389
H	3.336667	-0.066665	-0.552069
H	1.182282	0.022475	-1.794298
H	-0.958291	0.100150	-0.534558
H	-0.952425	0.090431	1.927103

B3PW91/6-31G* Structure 5 Z
Energy: -479.394901
# of imaginary frequencies = 0

C	-0.003195	-0.038002	-0.004371
C	0.011349	0.013707	1.390985
C	1.244436	0.053059	2.054251
C	2.434394	0.043860	1.332848
C	2.409938	-0.006309	-0.062232
C	1.188648	-0.048989	-0.729911
C	-1.277018	0.036940	2.184349
N	-1.500510	1.290049	2.885470
C	-1.300203	1.418600	4.230204
O	-0.986784	0.478006	4.948282
C	-1.509524	2.814214	4.787245
H	3.340378	-0.015503	-0.624393
H	3.385304	0.069719	1.859455
H	1.260507	0.082814	3.141380
H	1.160793	-0.090856	-1.816022
H	-0.955947	-0.074321	-0.530196
H	-2.130334	-0.161161	1.524370
H	-1.266099	-0.733318	2.961370
H	-1.635280	2.123525	2.332287
H	-2.267083	2.765750	5.575032
H	-0.578121	3.151119	5.252715
H	-1.820955	3.551192	4.040356

B3PW91/6-31G* Structure 6 Z
Energy: -710.354772
# of imaginary frequencies = 0

C	0.006387	0.012269	-0.000610
C	0.002422	-0.001711	1.397977
C	1.226619	-0.003536	2.076060
C	2.428195	0.007198	1.370603
C	2.421957	0.024675	-0.023687
C	1.207298	0.028035	-0.707586
C	-1.322696	-0.096971	2.145108
N	-1.633177	-1.493180	2.423162
C	-2.558757	-2.184982	1.688580
O	-3.282279	-1.650602	0.859969
C	-1.403406	0.777636	3.391006
C	-0.938445	2.098359	3.341342
C	-1.049939	2.935547	4.447534
C	-1.626475	2.466897	5.628131
C	-2.096003	1.157596	5.686214
C	-1.987951	0.321339	4.574672
C	-2.629122	-3.672340	1.976041
H	3.359394	0.039210	-0.573943
H	1.239510	0.005204	3.163853
H	3.371342	0.008427	1.911686
H	1.193112	0.044818	-1.794577
H	-0.940931	0.002201	-0.534965
H	-0.683564	3.957438	4.387344
H	-0.482614	2.471591	2.427684
H	-2.373560	-0.693110	4.621036
H	-2.553194	0.781646	6.598350
H	-2.121140	0.212202	1.459588
H	-0.964201	-2.017603	2.970019
H	-3.678752	-3.958834	2.080261
H	-2.224240	-4.218403	1.117106
H	-2.082455	-3.975454	2.874611
H	-1.710609	3.119197	6.493616

B3PW91/6-31G* Structure 7 Z
Energy: -287.731461
# of imaginary frequencies = 0

C	0.003792	0.001743	0.006703
C	0.004292	-0.005412	1.531676
C	1.419345	-0.005583	2.100012
O	2.337947	0.598396	1.562120
N	1.573390	-0.706866	3.261039
C	2.828056	-0.766153	3.974797
H	-0.489861	0.902283	1.906091
H	-0.573126	-0.854941	1.919921
H	-1.012207	0.122217	-0.383340
H	0.624544	0.822192	-0.362323
H	0.414200	-0.931838	-0.393148
H	0.771530	-1.179824	3.649129
H	3.560384	-0.214023	3.382953
H	3.170437	-1.801134	4.093133
H	2.750151	-0.304341	4.966954

B3PW91/6-31G* Structure 8 Z
Energy: -327.034348
# of imaginary frequencies = 0

C	0.004966	0.001197	0.008755
C	0.004904	0.001252	1.533860
C	1.419859	0.001199	2.103235
O	2.345881	-0.580989	1.553560
N	1.573879	0.688726	3.272763
C	2.819570	0.681425	4.017948
C	2.870708	-0.391209	5.103287
H	-0.571655	0.849166	1.926315
H	-0.489250	-0.908552	1.903638
H	0.409291	0.939585	-0.385695
H	-1.010044	-0.124250	-0.382272
H	0.631895	-0.812822	-0.363907
H	0.753371	1.077550	3.714091
H	3.612617	0.514195	3.284540
H	2.969230	1.677569	4.451891
H	2.766210	-1.386413	4.659768
H	3.827362	-0.352696	5.637013
H	2.069412	-0.256132	5.839691

B3PW91/6-31G* Structure 9 Z
Energy: -366.336912
# of imaginary frequencies = 0

C	-0.005892	-0.030338	0.000293
C	0.016079	0.006652	1.524518
C	1.438644	-0.028410	2.074836
O	2.377177	0.499413	1.491298
N	1.581301	-0.675937	3.267052
C	2.839875	-0.716097	4.000731
C	3.044951	-2.101881	4.608425
C	2.909942	0.395096	5.050824
H	-0.441461	0.941450	1.878772
H	-0.583175	-0.811148	1.945975
H	-1.021905	0.118791	-0.379736
H	0.362050	-0.990704	-0.376549
H	0.641718	0.753311	-0.401008
H	0.754473	-1.032707	3.725507
H	3.609350	-0.530677	3.244693
H	2.784848	1.374397	4.578596
H	3.877921	0.383723	5.565152
H	2.125168	0.273257	5.808448
H	4.008975	-2.156226	5.125557
H	2.264125	-2.332391	5.345929
H	3.024621	-2.876751	3.835181

B3PW91/6-31G* Structure 10 Z
Energy: -327.032041
# of imaginary frequencies = 0

C	0.007449	0.009672	0.014980
C	-0.000688	-0.002820	1.546911
C	1.440780	-0.006505	2.056760
O	2.212554	-0.921079	1.795368
C	-0.728432	-1.237341	2.088696
N	1.798115	1.071141	2.813109
C	3.122016	1.227358	3.370954
H	-0.517204	0.899381	1.906709
H	-0.199684	-2.144423	1.779908
H	-1.753502	-1.280698	1.703646
H	-0.775748	-1.228716	3.183606
H	0.489273	0.912215	-0.378081
H	0.558277	-0.858574	-0.360013
H	-1.015385	-0.028345	-0.376409
H	1.110148	1.788049	2.985542
H	3.091620	1.275115	4.466229
H	3.612355	2.132044	2.991528
H	3.702188	0.353771	3.068006

B3PW91/6-31G* Structure 11 Z
Energy: -366.334936
# of imaginary frequencies = 0

C	-0.025706	0.055323	0.012453
C	-0.001371	-0.013587	1.542630
C	1.450747	-0.029694	2.022033
O	2.226435	-0.918040	1.689922
C	-0.712725	-1.270747	2.053898
N	1.815632	1.008280	2.828972
C	3.137604	1.122542	3.415210
C	3.154314	0.829235	4.912839
H	-0.513379	0.872601	1.945864
H	-1.745387	-1.304944	1.688862
H	-0.187294	-2.163770	1.701359
H	-0.737808	-1.302545	3.149260
H	0.435842	0.978529	-0.355995
H	-1.055889	0.017222	-0.359370
H	0.529047	-0.790547	-0.405342
H	1.111086	1.679180	3.097819
H	3.764341	0.407223	2.876593
H	3.531465	2.128081	3.217387
H	2.809161	-0.191021	5.108958
H	4.169866	0.931306	5.312222
H	2.507496	1.521396	5.465826

B3PW91/6-31G* Structure 12 Z
Energy: -405.637501
# of imaginary frequencies = 0

C	0.060290	-0.306059	-0.019555
C	0.023314	0.018685	1.477042
C	1.446448	-0.026188	2.036179
O	2.120725	-1.048671	1.987654
C	-0.848142	-0.982664	2.242188
N	1.898860	1.136302	2.586451
C	3.226088	1.286330	3.167834
C	3.128478	1.661368	4.646975
C	4.057930	2.292951	2.371689
H	-0.394672	1.027251	1.611211
H	-0.418272	-1.985960	2.161712
H	-1.864115	-1.002802	1.831956
H	-0.915424	-0.726961	3.305866
H	-0.953396	-0.328485	-0.435385
H	0.641060	0.436805	-0.578306
H	0.524301	-1.284972	-0.175007
H	1.288206	1.941158	2.584254
H	3.677068	0.293485	3.075187
H	3.607751	3.293935	2.404982
H	5.069997	2.371291	2.784627
H	4.137234	1.988254	1.323355
H	2.555172	0.911792	5.201659
H	2.637230	2.634749	4.777861
H	4.126124	1.732200	5.094722

B3PW91/6-31G* Structure 13 Z
Energy: -518.693108
# of imaginary frequencies = 0

C	0.019699	-0.024209	-0.012557
C	0.020591	-0.034436	1.380422
C	1.234708	-0.026513	2.067454
C	2.438726	-0.006831	1.368285
C	2.448679	0.004679	-0.032405
C	1.226351	-0.006755	-0.711373
C	3.761073	0.051656	-0.800382
C	4.691754	-1.065072	-0.307411
N	4.521134	-2.263385	-0.932985
C	5.218008	-3.460427	-0.518908
C	4.455267	1.411102	-0.672628
O	5.509515	-0.889764	0.587325
H	-0.920512	-0.030259	-0.558760
H	1.217532	0.006525	-1.800185
H	1.244695	-0.038215	3.154673
H	-0.918339	-0.049209	1.928073
H	3.383615	-0.014547	1.905698
H	3.534656	-0.128051	-1.860633
H	4.762503	1.583856	0.361789
H	3.778114	2.214049	-0.980658
H	5.353480	1.449408	-1.298388
H	3.759780	-2.352194	-1.589508
H	4.561042	-4.144998	0.033047
H	6.032573	-3.151118	0.138110
H	5.631822	-3.987329	-1.385508

B3PW91/6-31G* Structure 14 Z
Energy: -557.996121
# of imaginary frequencies = 0

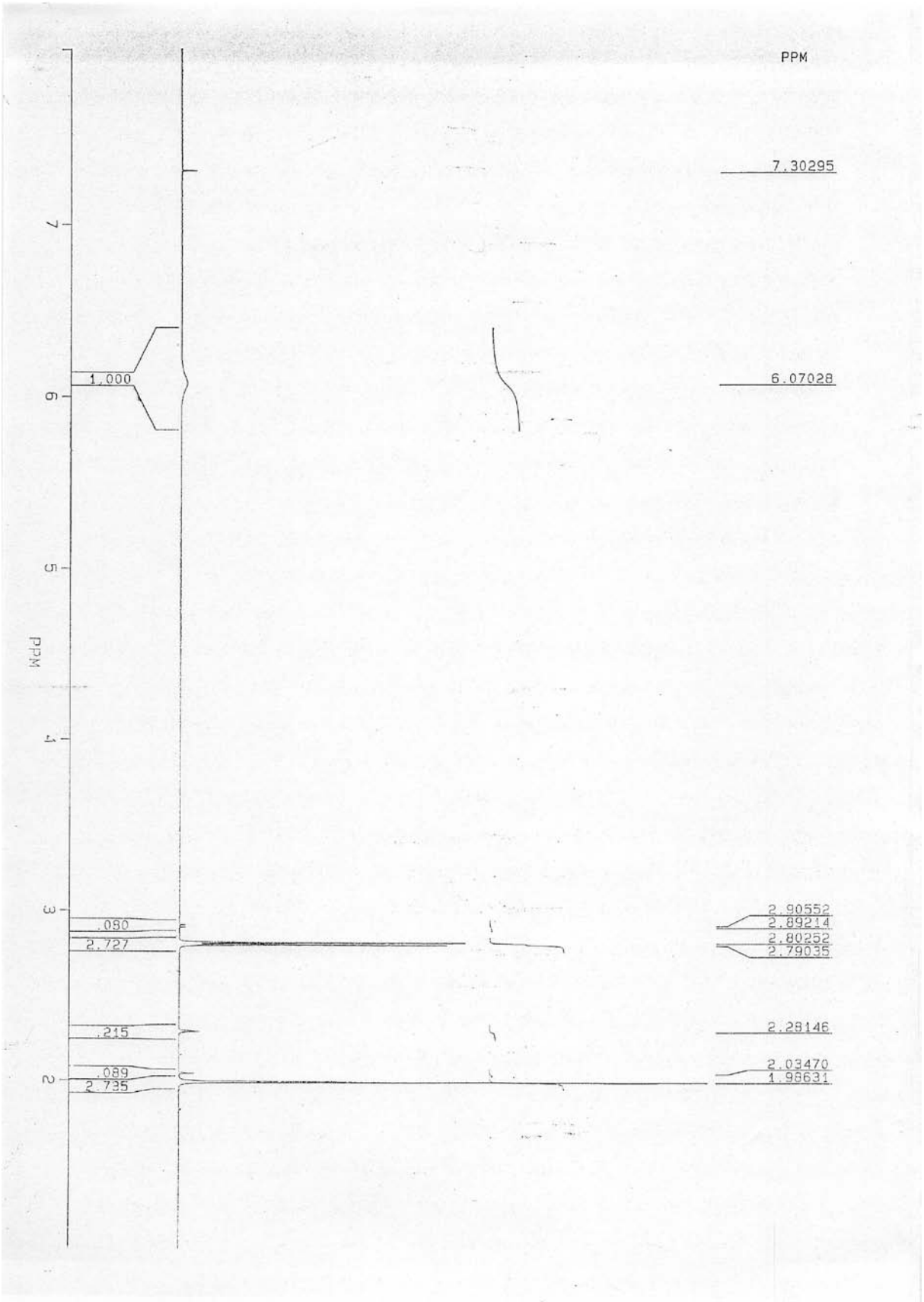
C	-0.024416	0.008798	0.009557
C	-0.017738	0.000209	1.410361
C	1.212507	-0.020358	2.074489
C	2.410734	-0.027278	1.361182
C	2.393389	-0.017223	-0.031680
C	1.171279	-0.000361	-0.704152
C	-1.320472	0.039678	2.195283
C	-2.014365	1.401311	2.088644
C	-2.260016	-1.069905	1.703112
O	-3.070733	-0.889487	0.802556
N	-2.112728	-2.265989	2.339898
C	-2.802249	-3.468373	1.907546
C	-1.945516	-4.368117	1.020629
H	3.357451	-0.040676	1.895907
H	1.234193	-0.022184	3.163140
H	1.148364	0.004007	-1.791238
H	3.325782	-0.023246	-0.590563
H	-0.975915	0.009840	-0.516111
H	-1.081114	-0.150245	3.250787
H	-2.330199	1.584990	1.058723
H	-1.333950	2.200601	2.399084
H	-2.907043	1.433824	2.722703
H	-1.340405	-2.366464	2.983299
H	-3.142996	-4.014085	2.796179
H	-3.688074	-3.129671	1.364438
H	-1.041932	-4.704288	1.543242
H	-1.637915	-3.833736	0.116387
H	-2.509453	-5.258557	0.719823

B3PW91/6-31G* Structure 15 Z
Energy: -597.298671
# of imaginary frequencies = 0

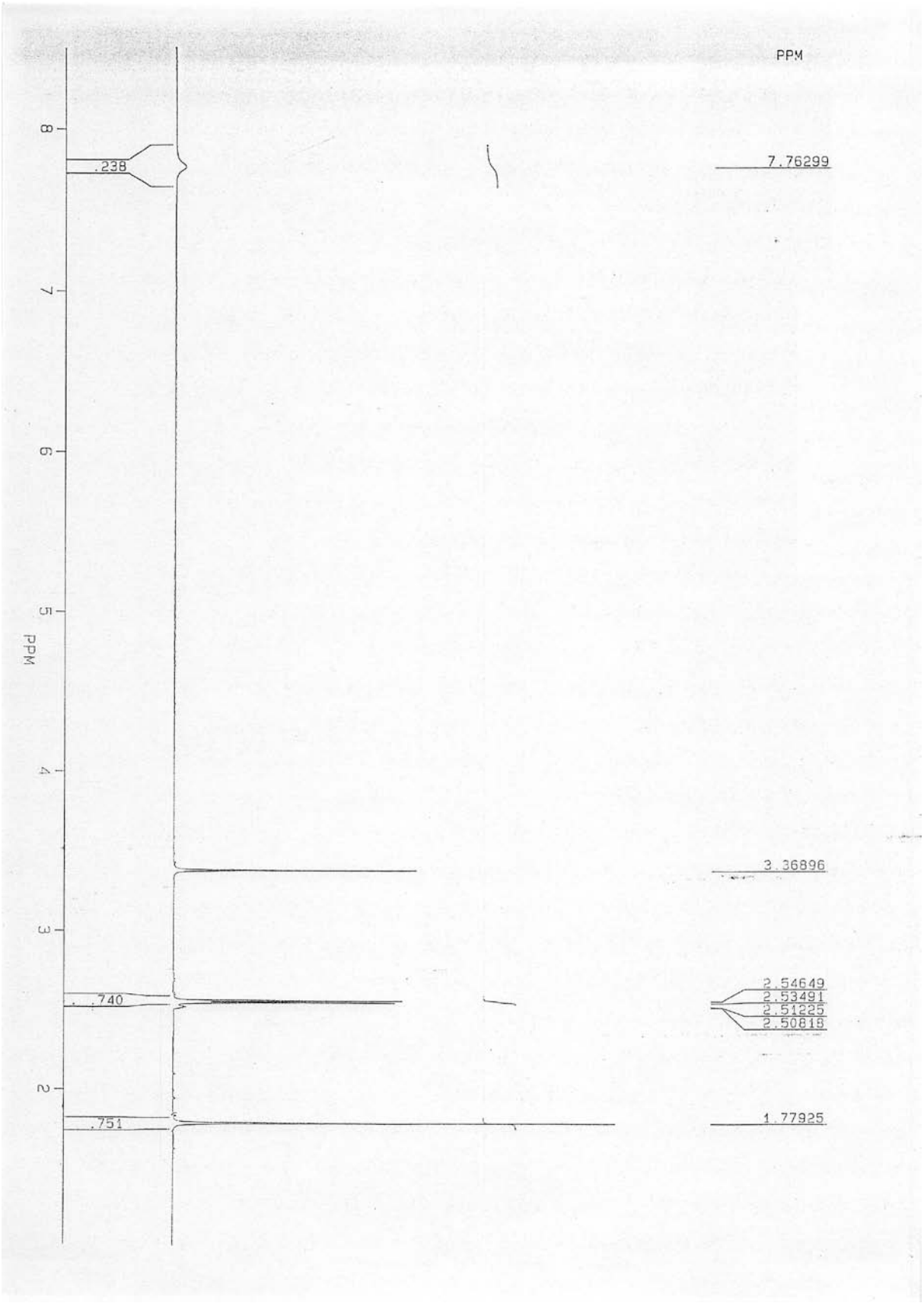
C	-0.017491	0.018560	0.021995
C	-0.005324	0.016097	1.414488
C	1.207173	-0.000902	2.115850
C	2.401449	-0.018588	1.388846
C	2.390892	-0.013572	-0.005571
C	1.179832	0.005135	-0.693724
C	1.228233	0.024718	3.636634
C	0.330220	-1.090659	4.190560
N	0.959285	-2.278623	4.406798
C	0.243350	-3.489149	4.794059
C	-0.225282	-4.277410	3.569101
C	0.783802	1.380636	4.194953
O	-0.863002	-0.918964	4.413029
C	1.114299	-4.326609	5.726883
H	3.330496	-0.024727	-0.552749
H	3.352098	-0.027875	1.919762
H	-0.967441	0.029317	-0.506990
H	1.168012	0.008335	-1.780740
H	-0.939278	0.013757	1.970536
H	2.260743	-0.166051	3.960401
H	-0.266523	1.562559	3.954093
H	1.390869	2.185275	3.768157
H	0.885753	1.404602	5.285444
H	1.910033	-2.380223	4.078116
H	-0.637795	-3.133742	5.337548
H	0.628068	-4.626799	2.974189
H	-0.856524	-3.651005	2.931708
H	-0.807141	-5.155505	3.872480
H	2.025253	-4.670260	5.218318
H	0.571328	-5.216935	6.061519
H	1.411327	-3.751584	6.610028

^{1}H-NMR spectra from amides **1-15** in $CDCl_3$, DMSO-d_6 and D_2O.

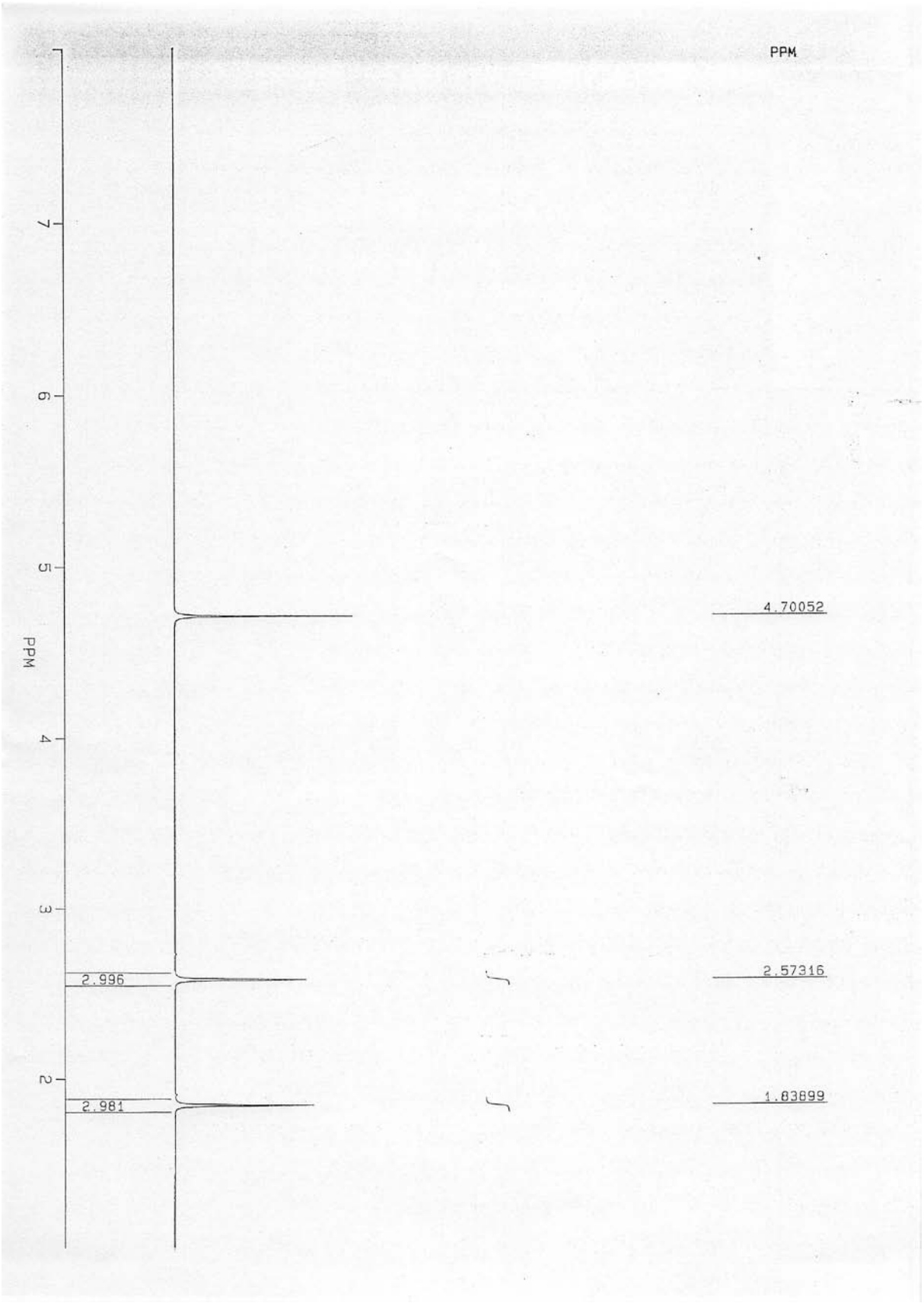
Compound **1**: $CDCl_3$



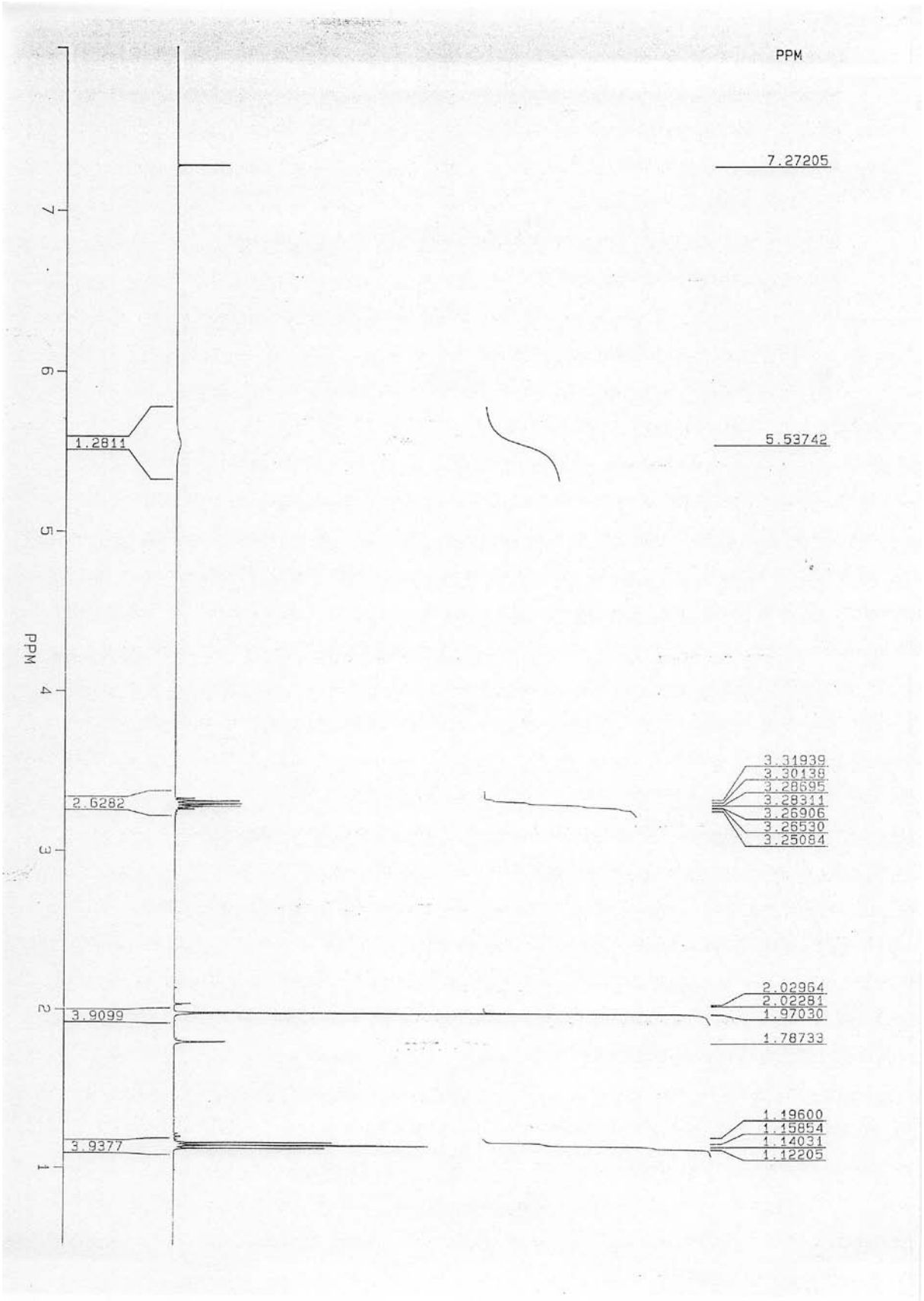
Compound **1**: DMSO-d_6



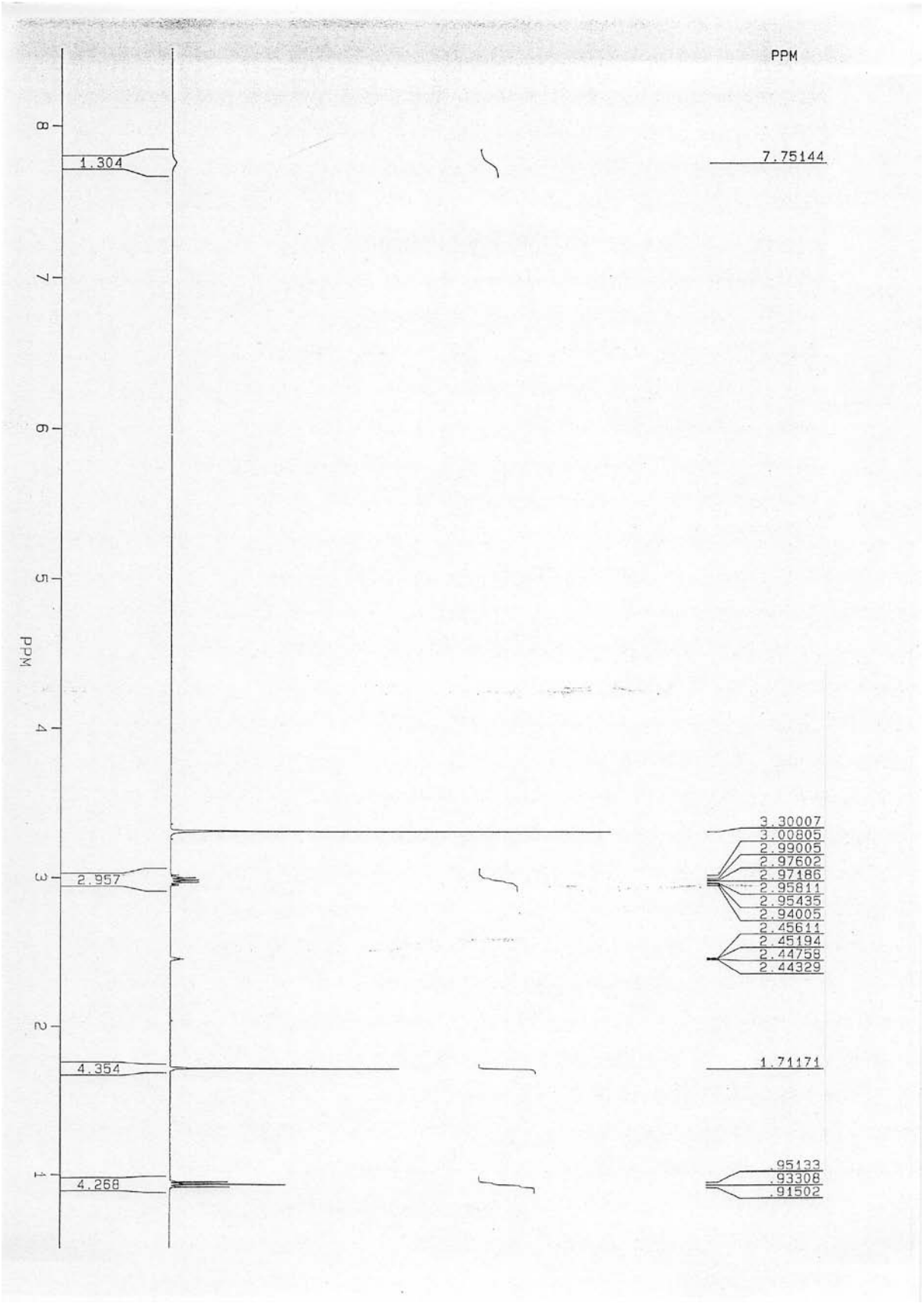
Compound **1**: D_2O



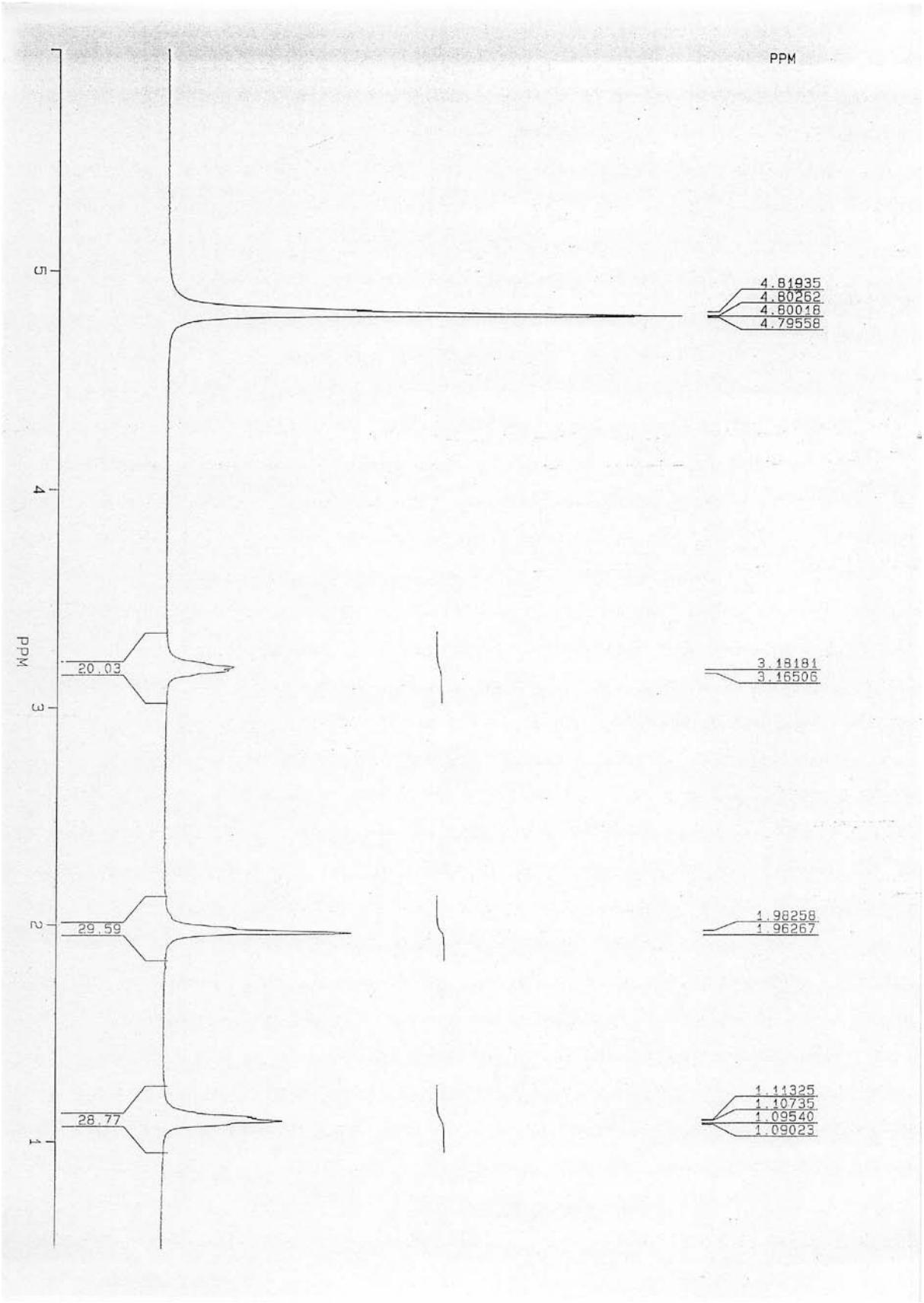
Compound **2**: $CDCl_3$



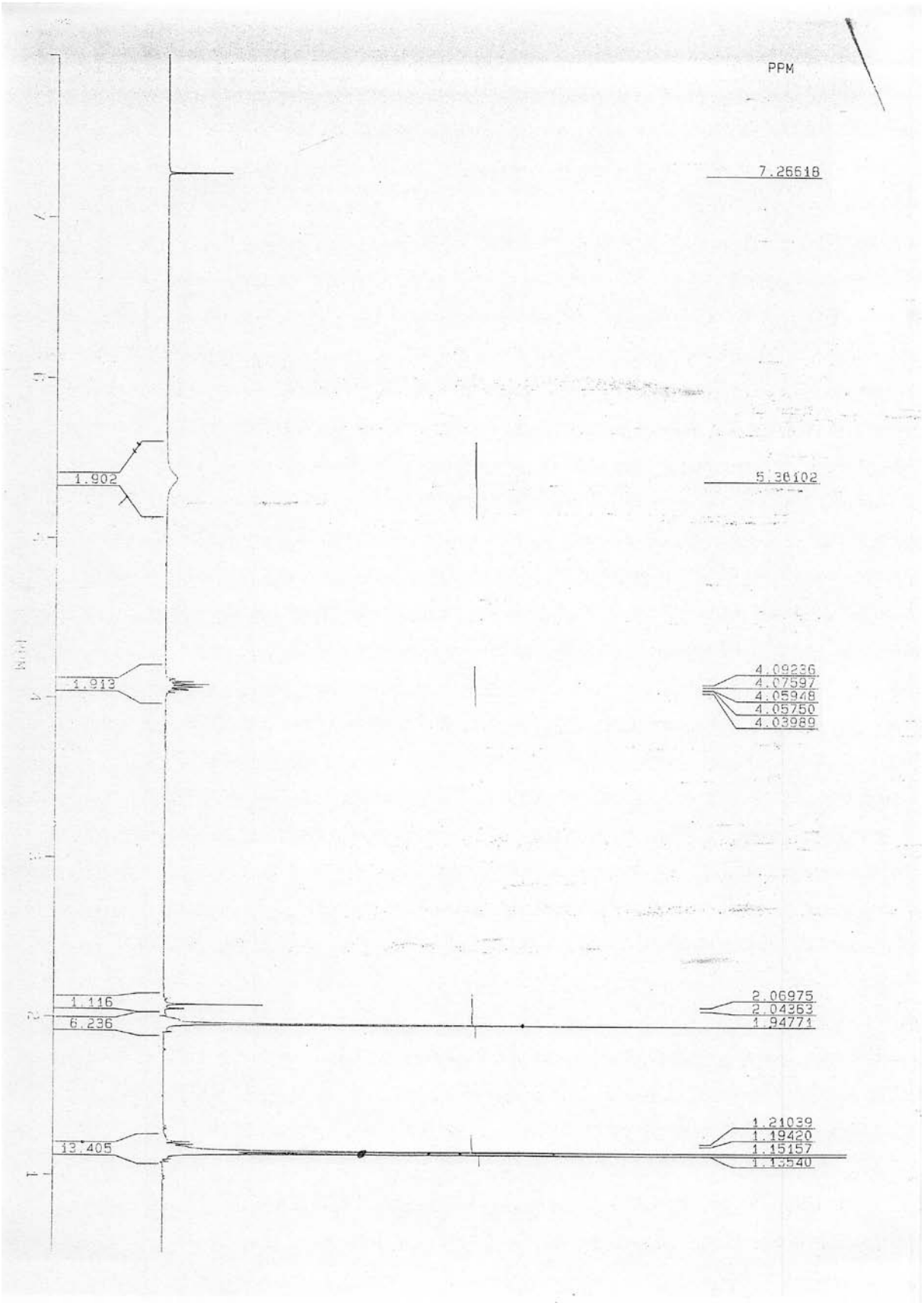
Compound **2**: DMSO-d_6



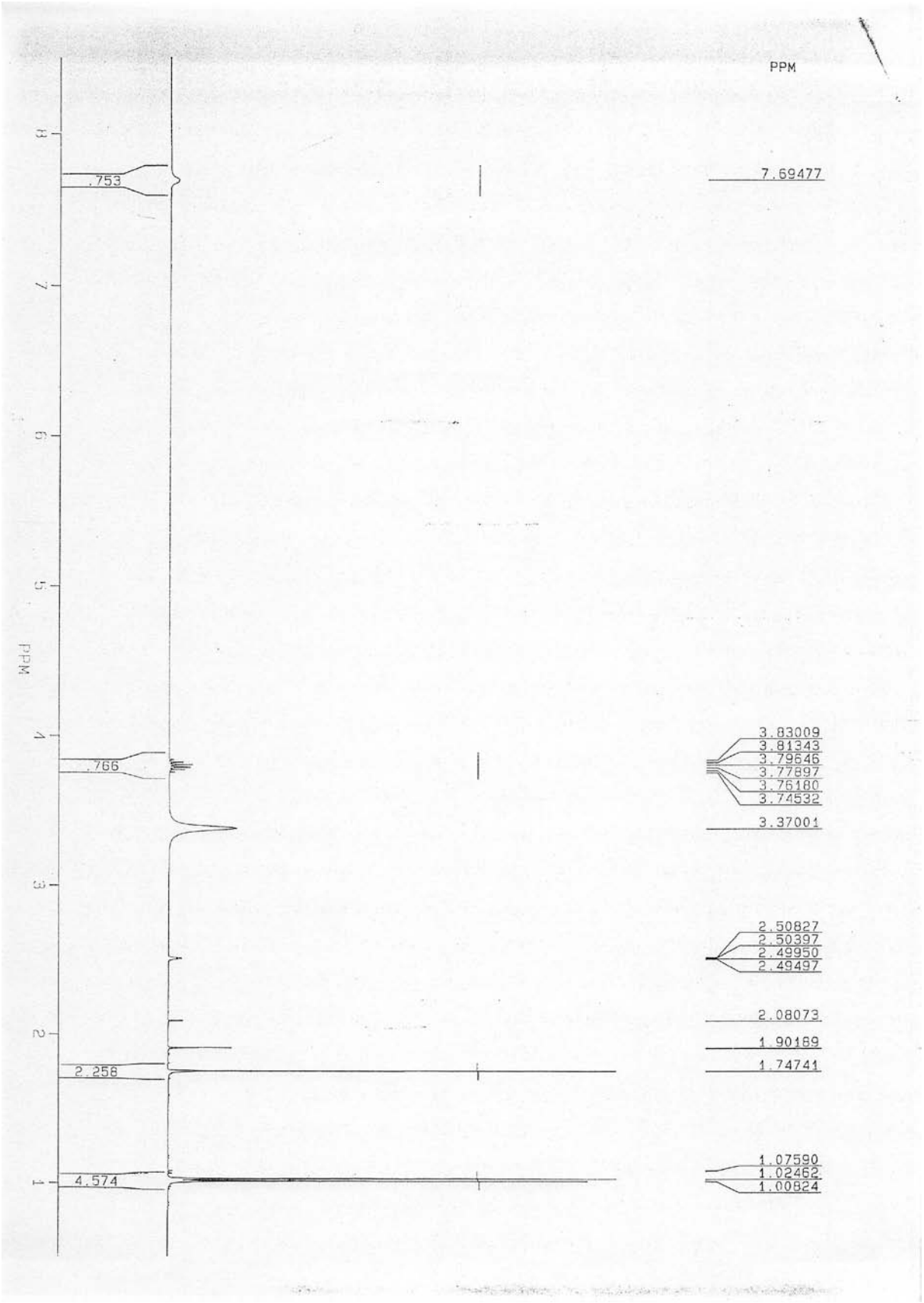
Compound **2**: D_2O



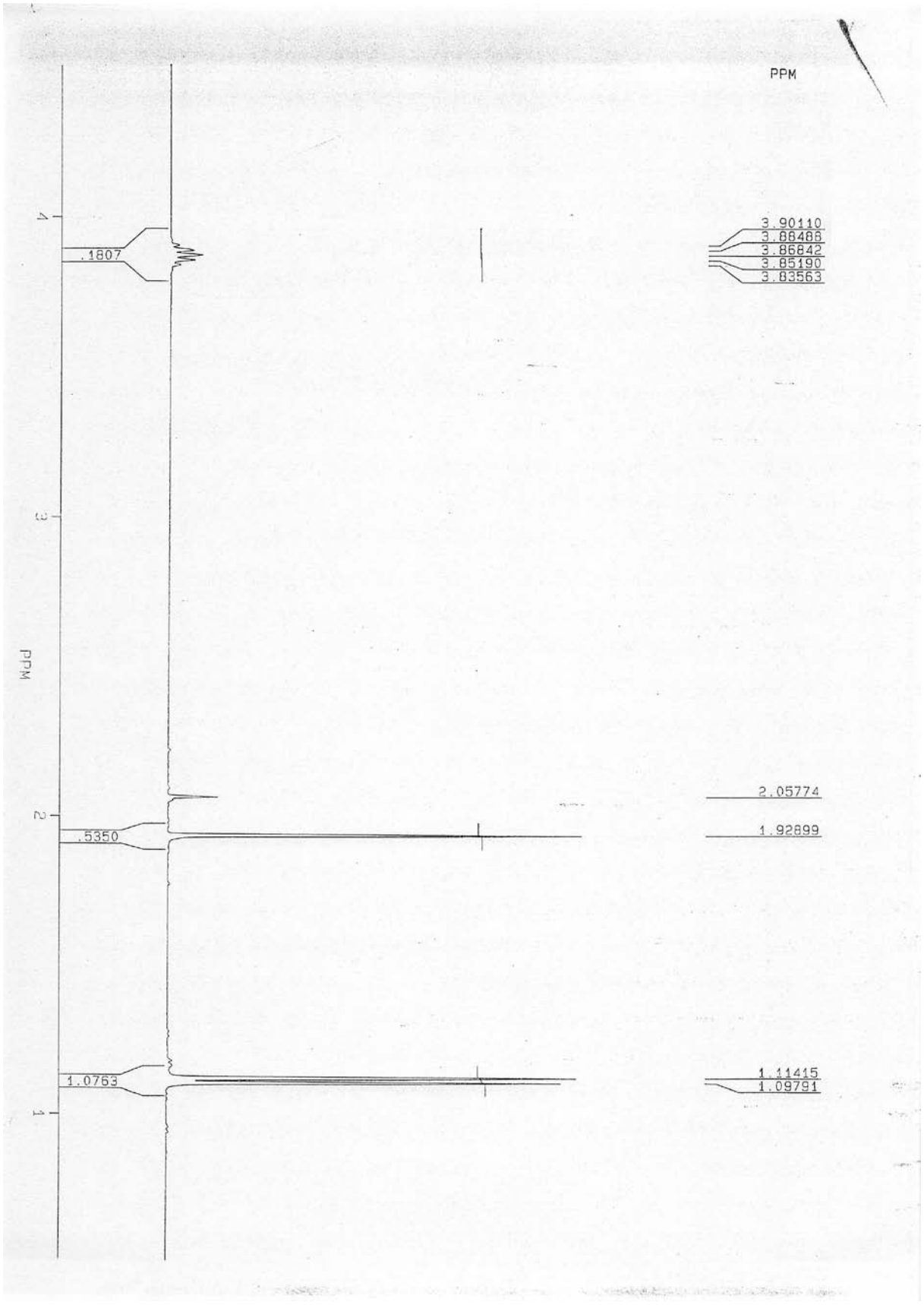
Compound **3**: $CDCl_3$



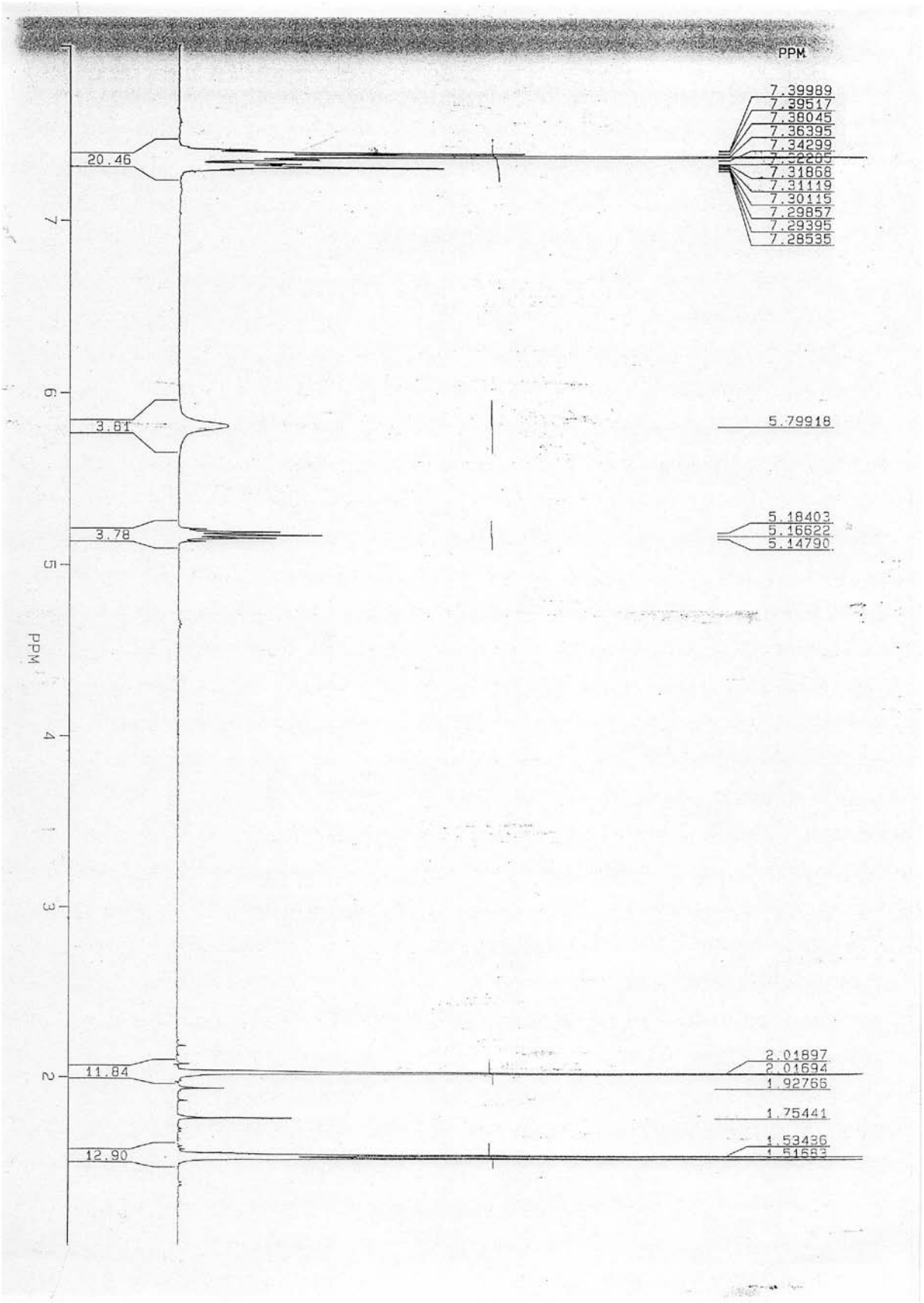
Compound **3**: DMSO-d_6



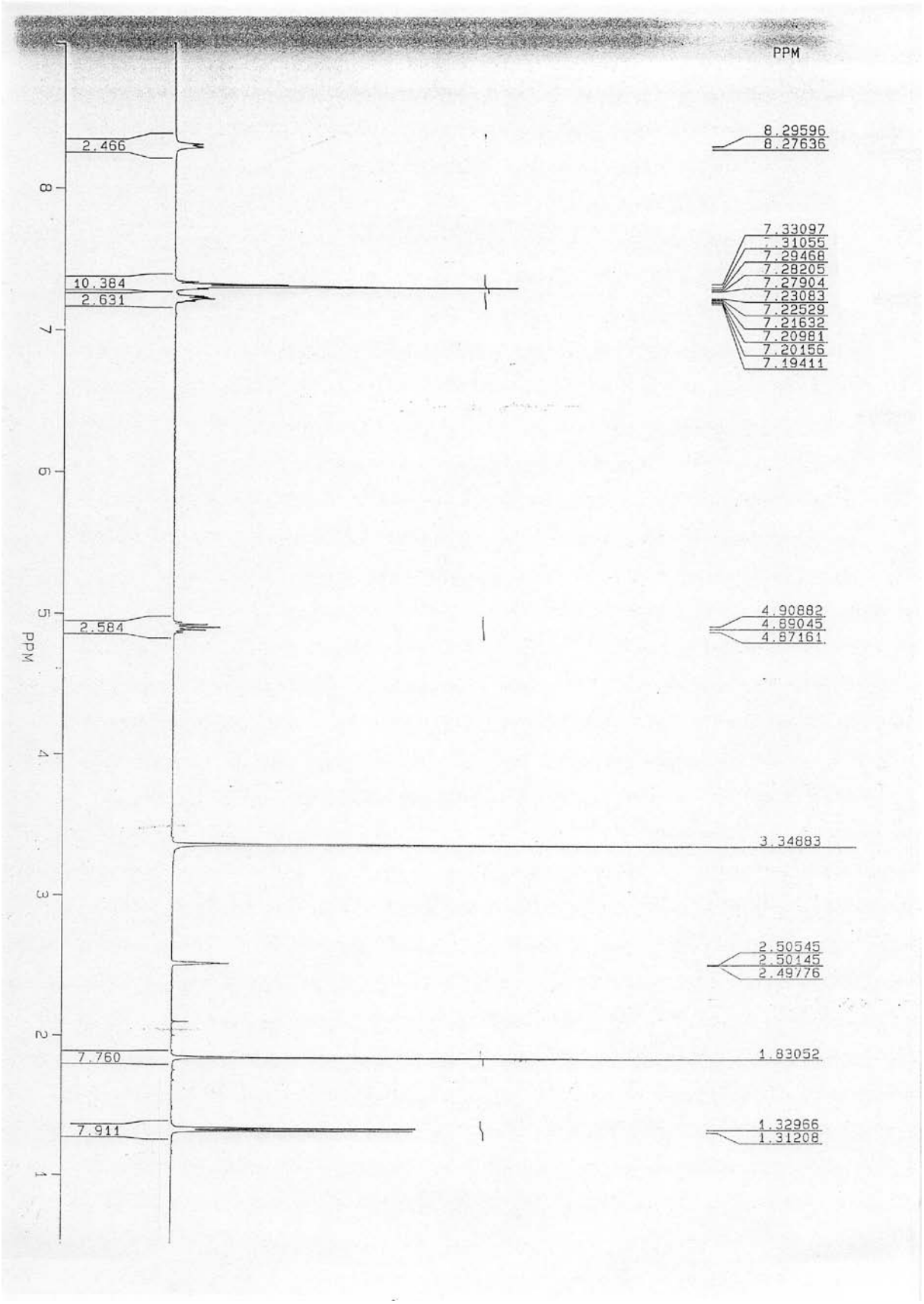
Compound **3**: D_2O



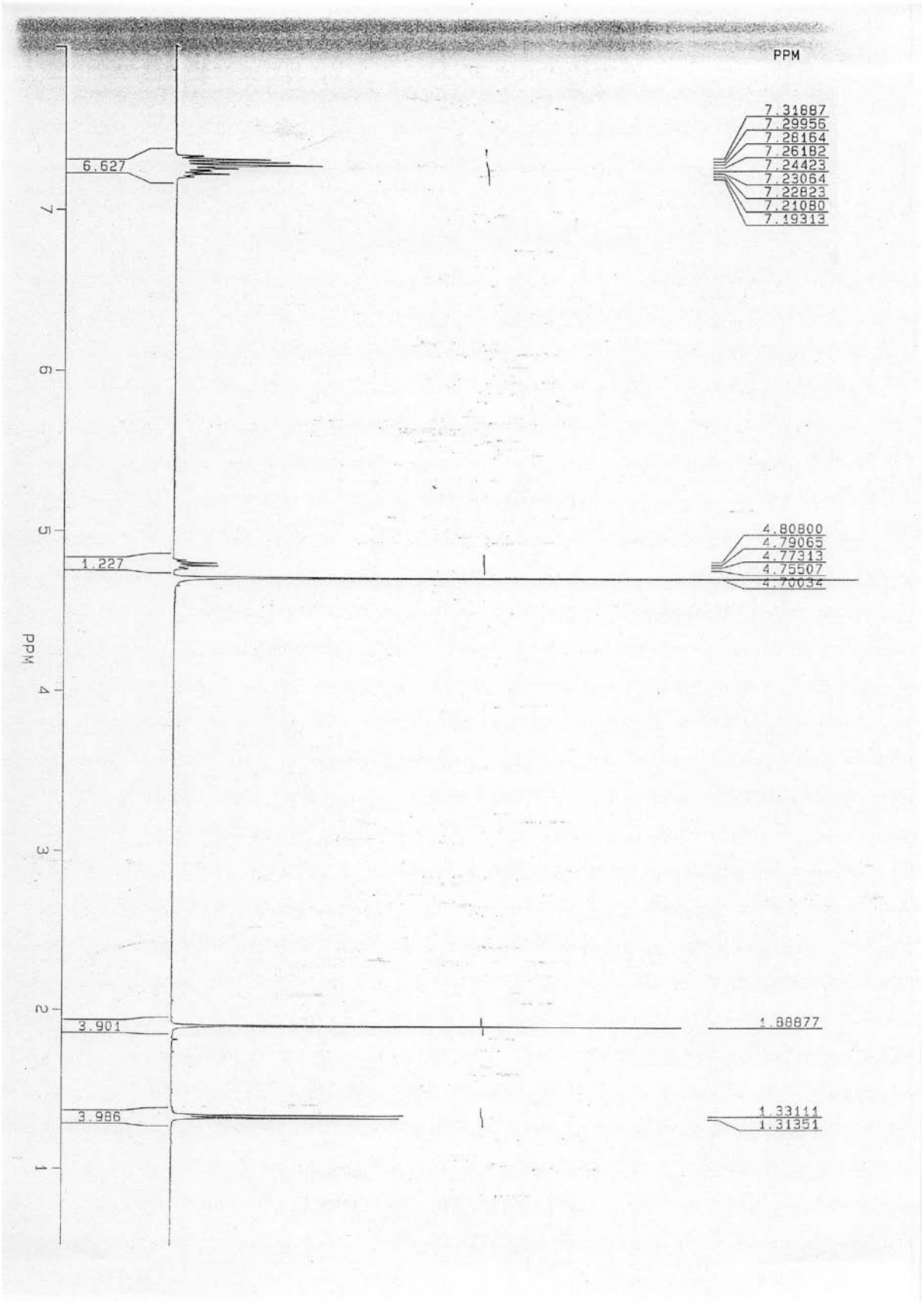
Compound **4**: $CDCl_3$



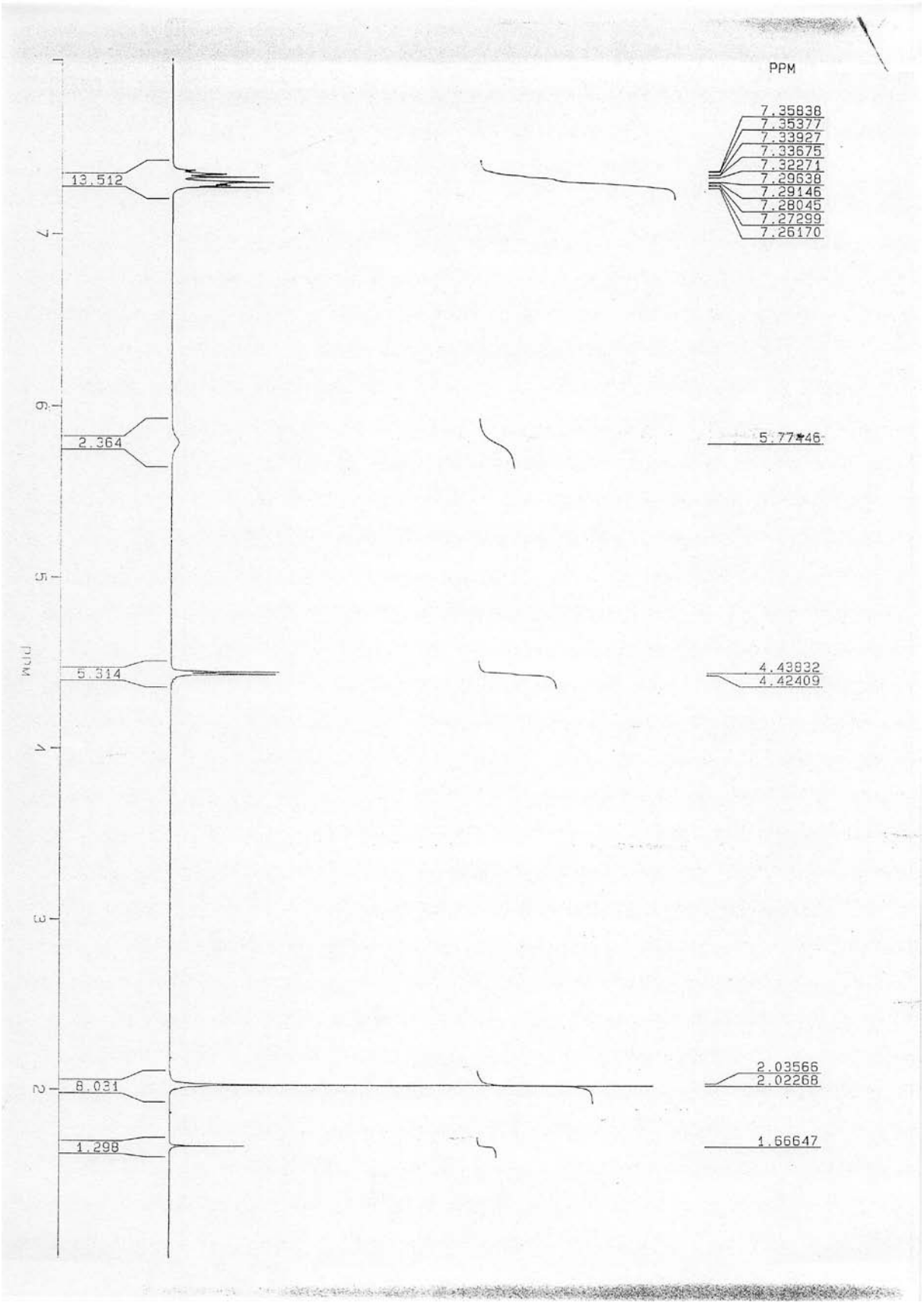
Compound **4**: DMSO-d_6



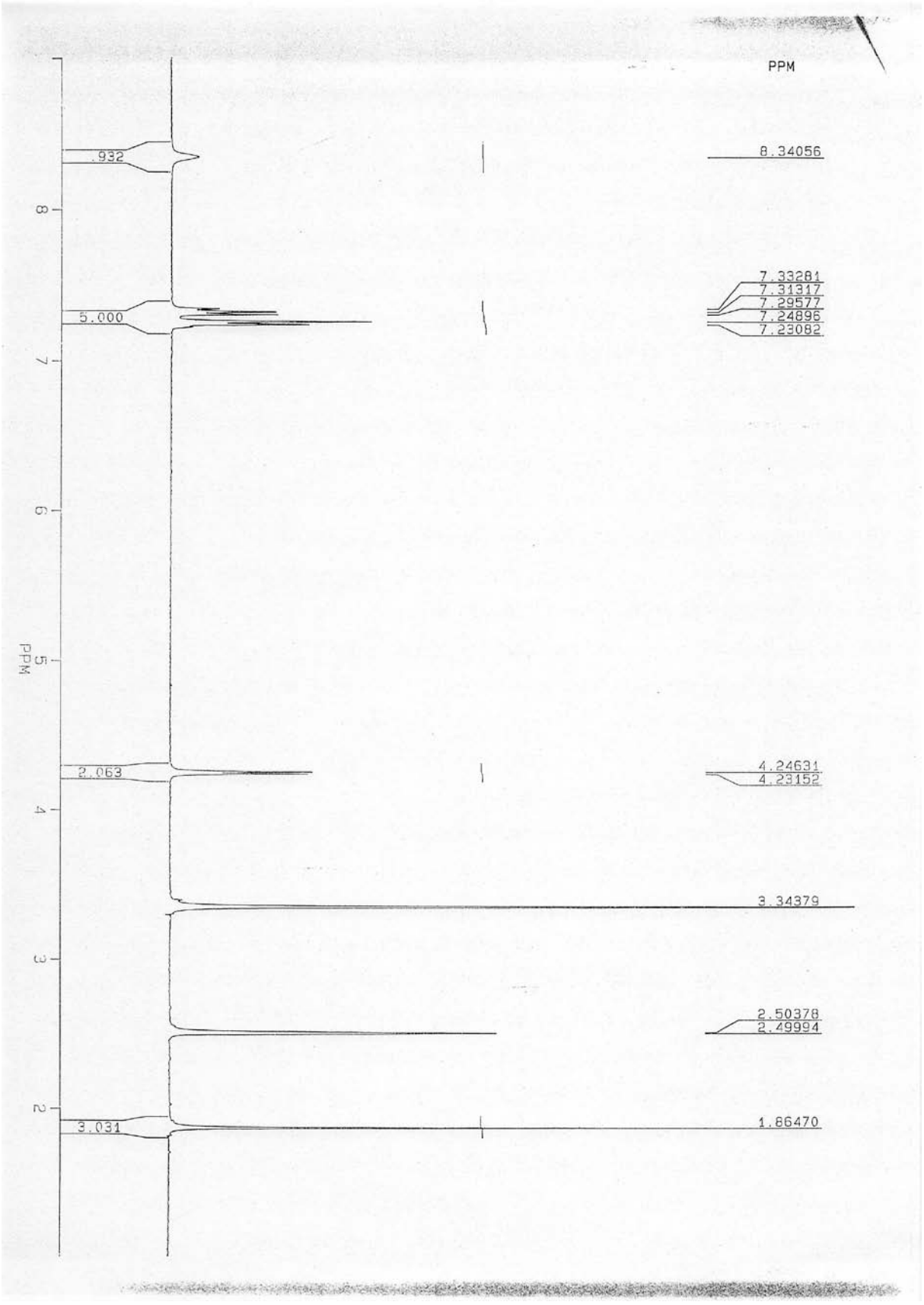
Compound **4**: D_2O



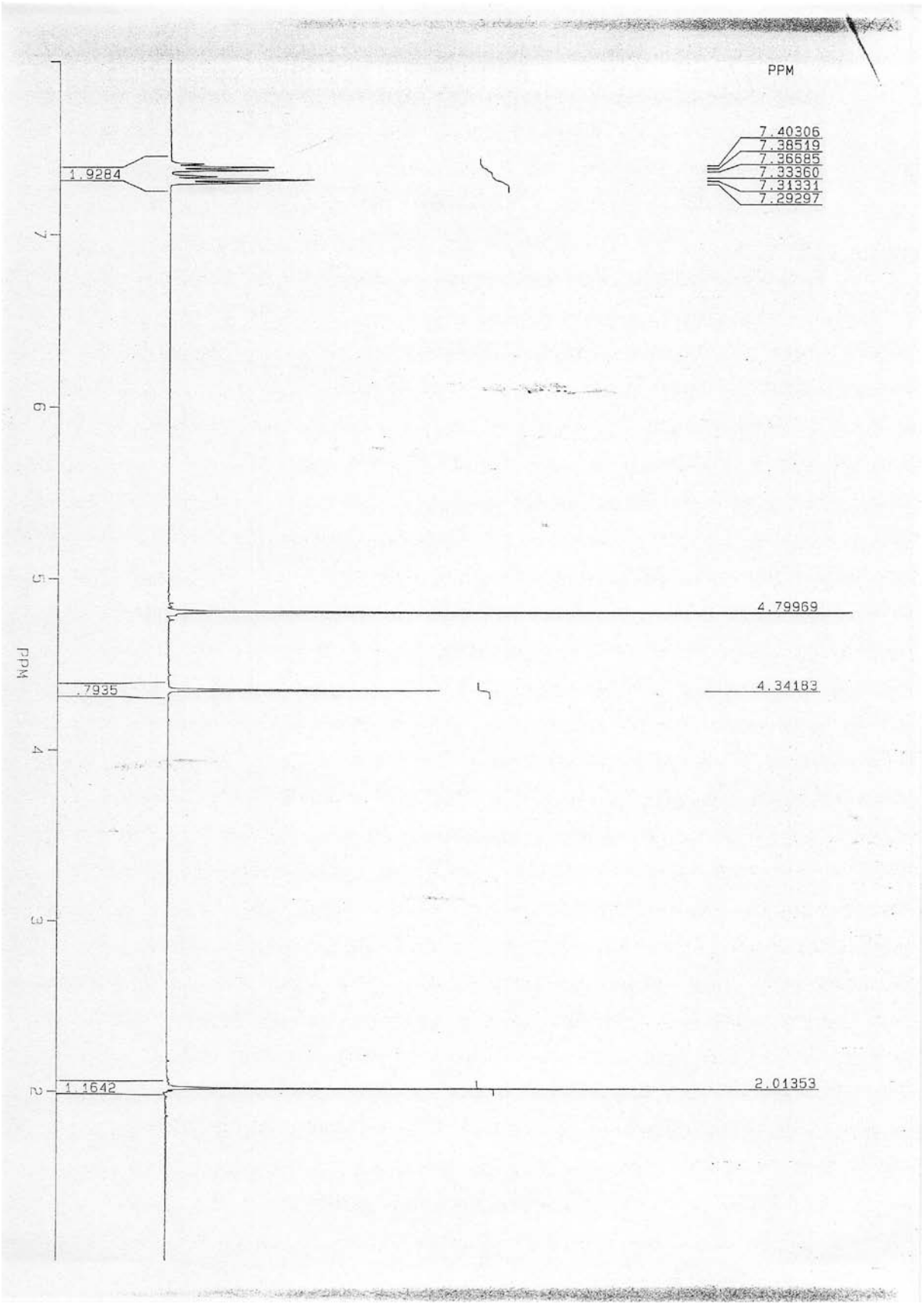
Compound **5**: $CDCl_3$



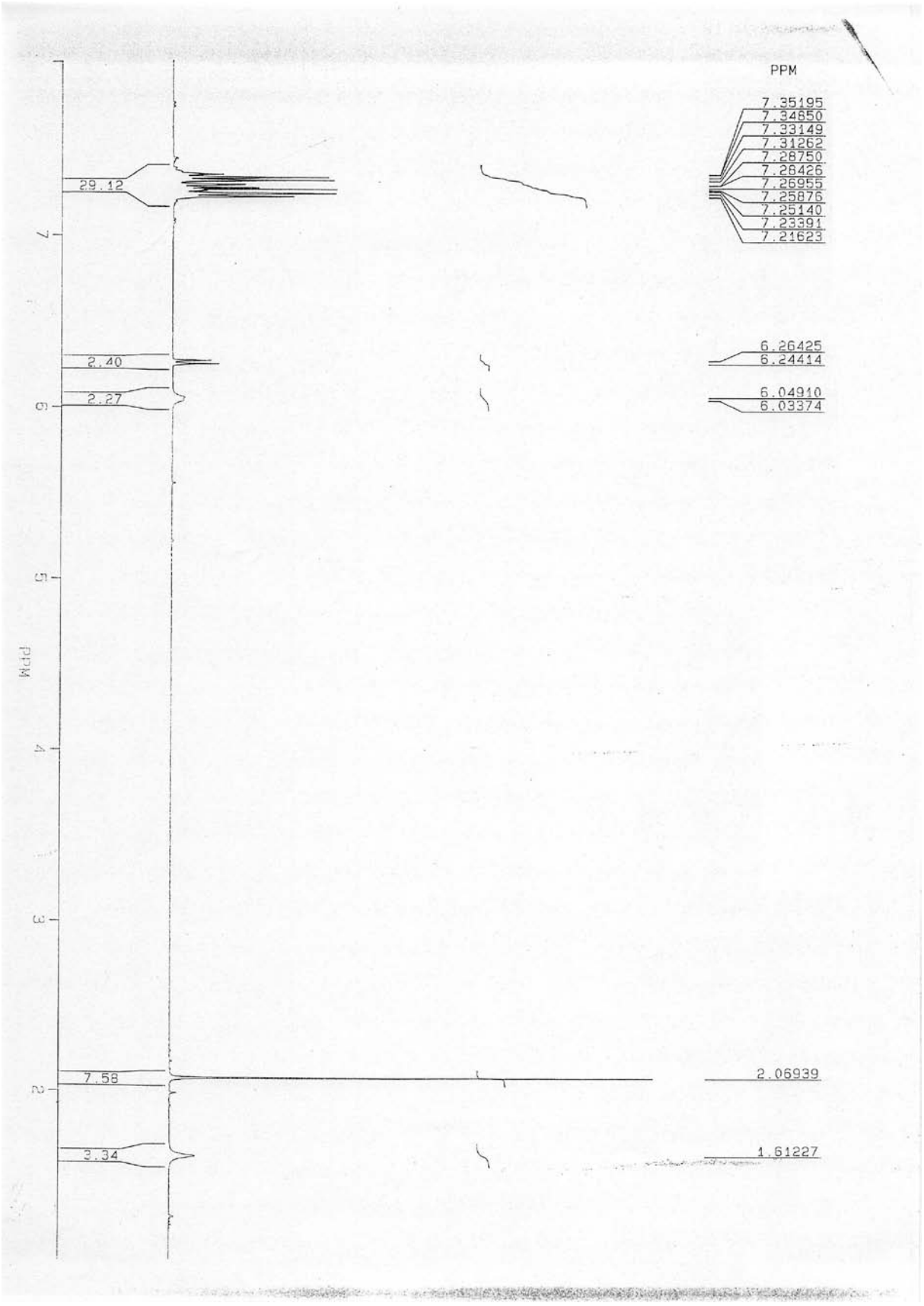
Compound **5**: DMSO-d_6



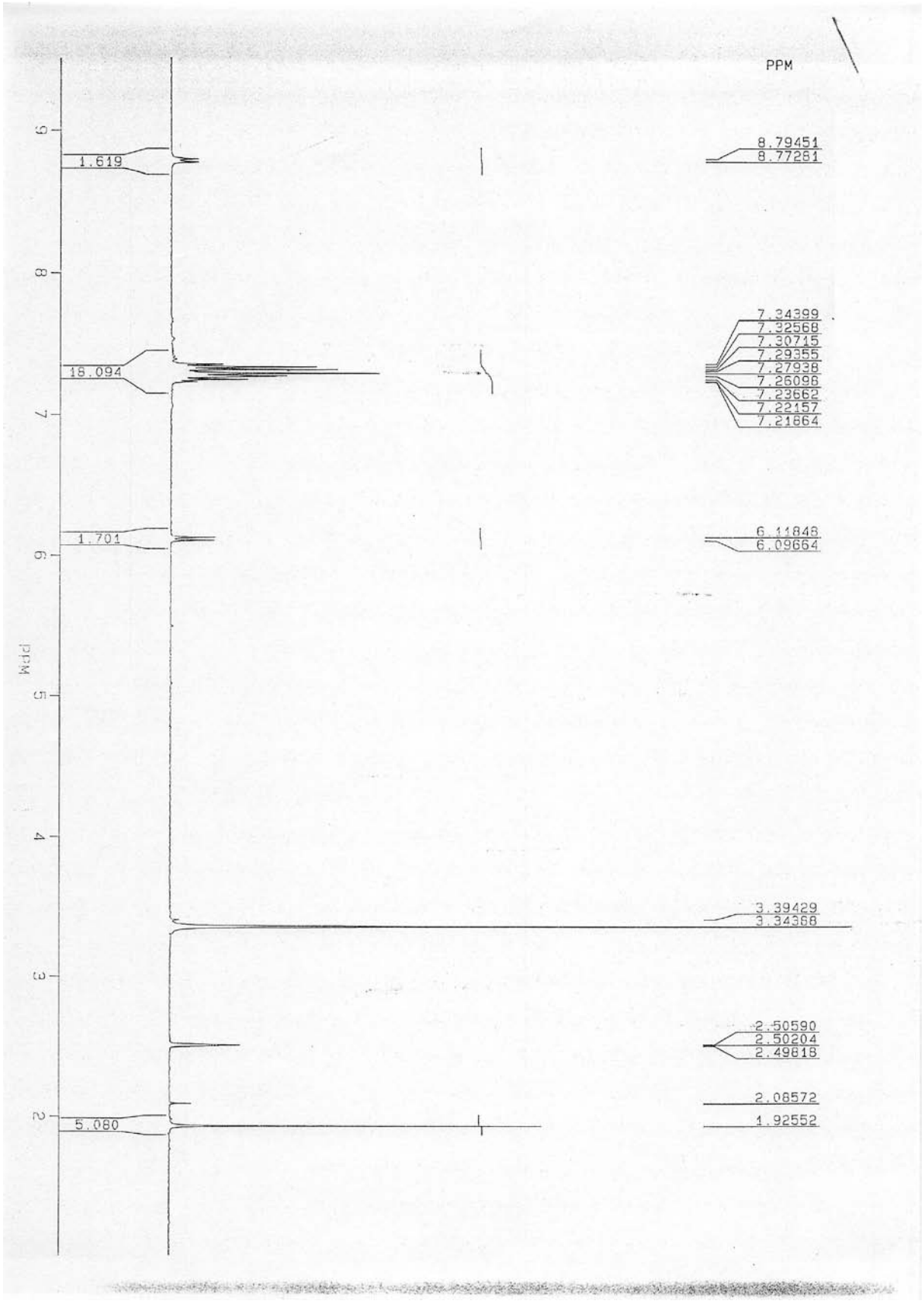
Compound **5**: D_2O



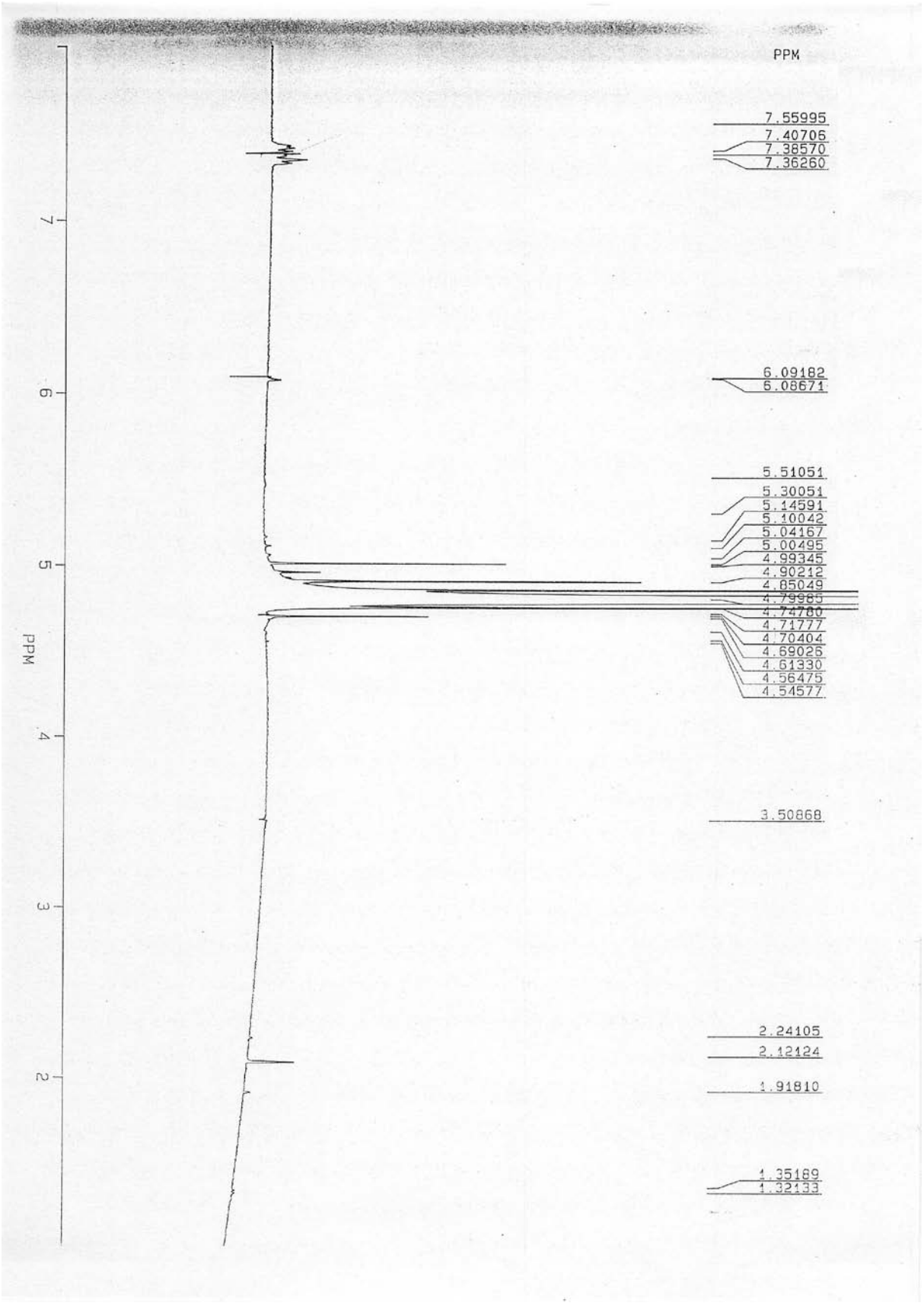
Compound **6**: $CDCl_3$



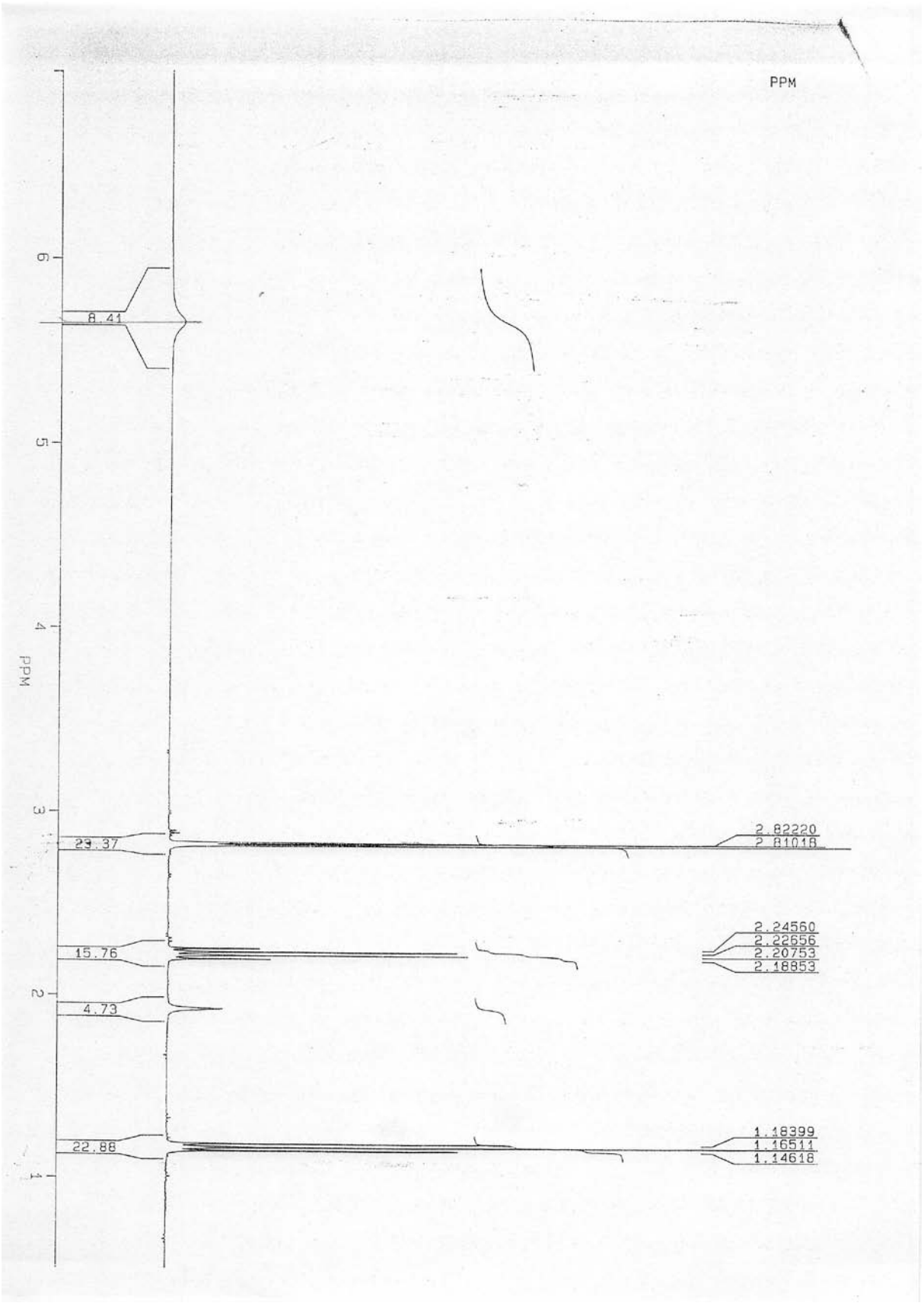
Compound **6**: DMSO-d_6



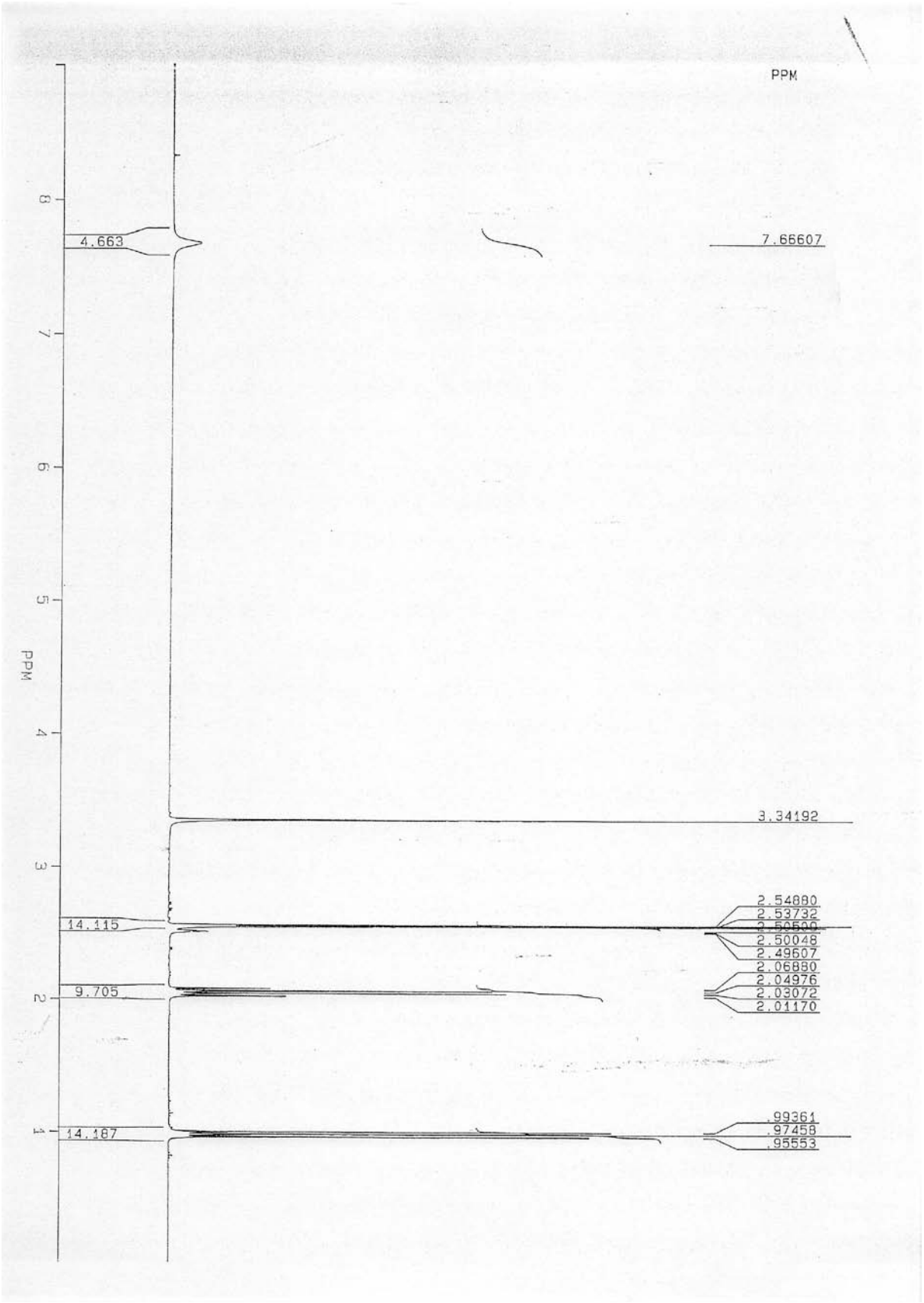
Compound **6**: D_2O



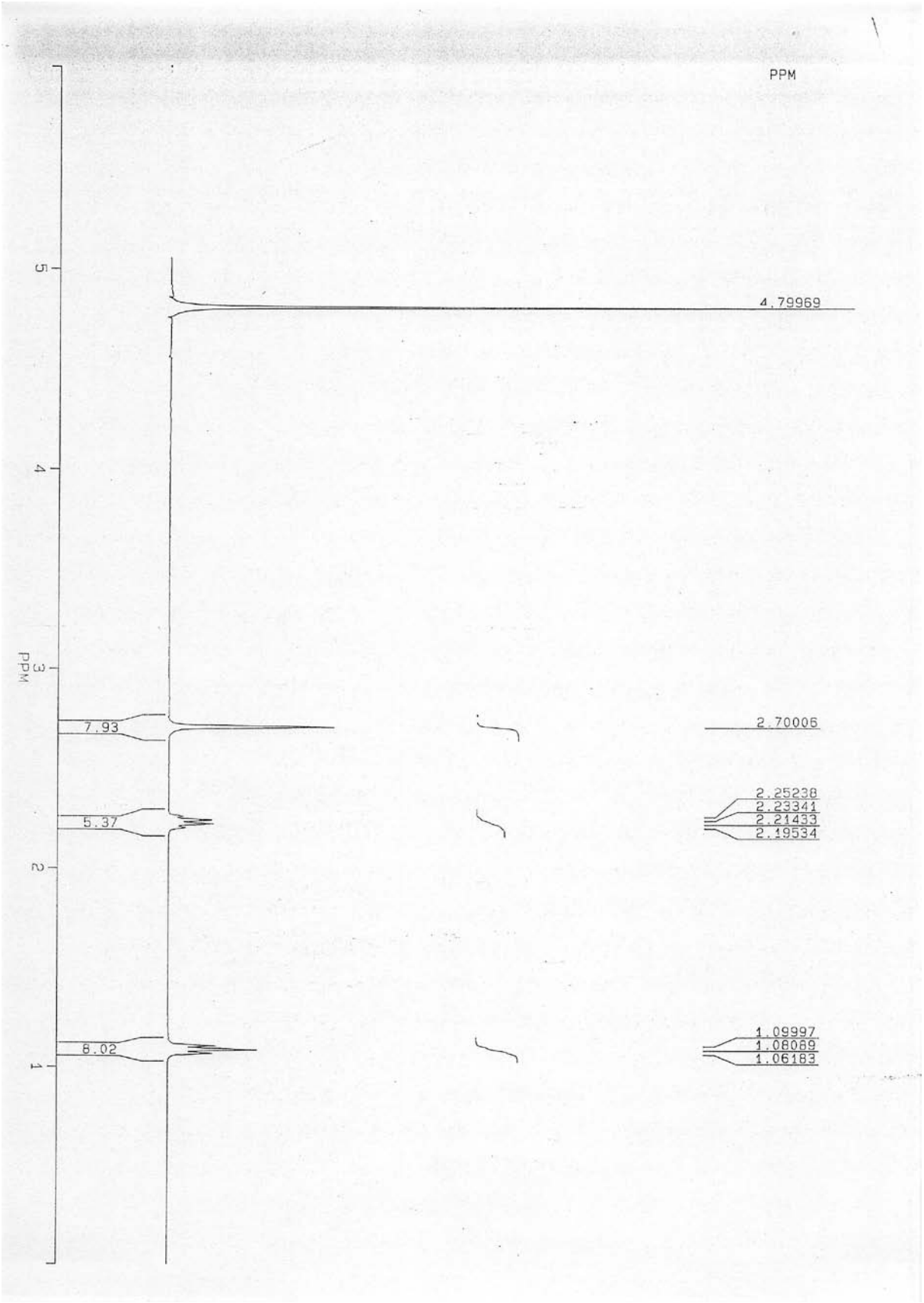
Compound **7**: $CDCl_3$



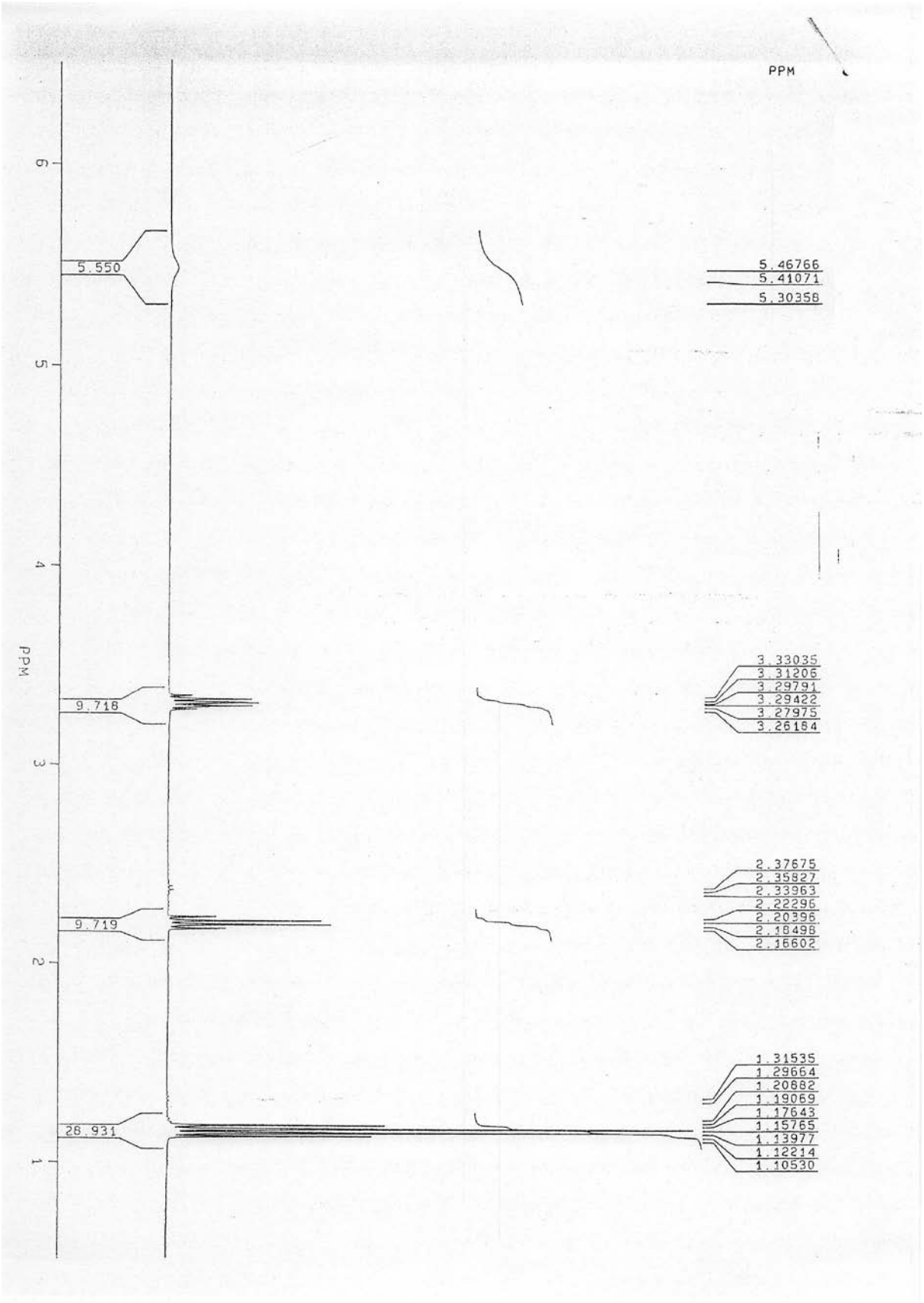
Compound **7**: DMSO-d_6



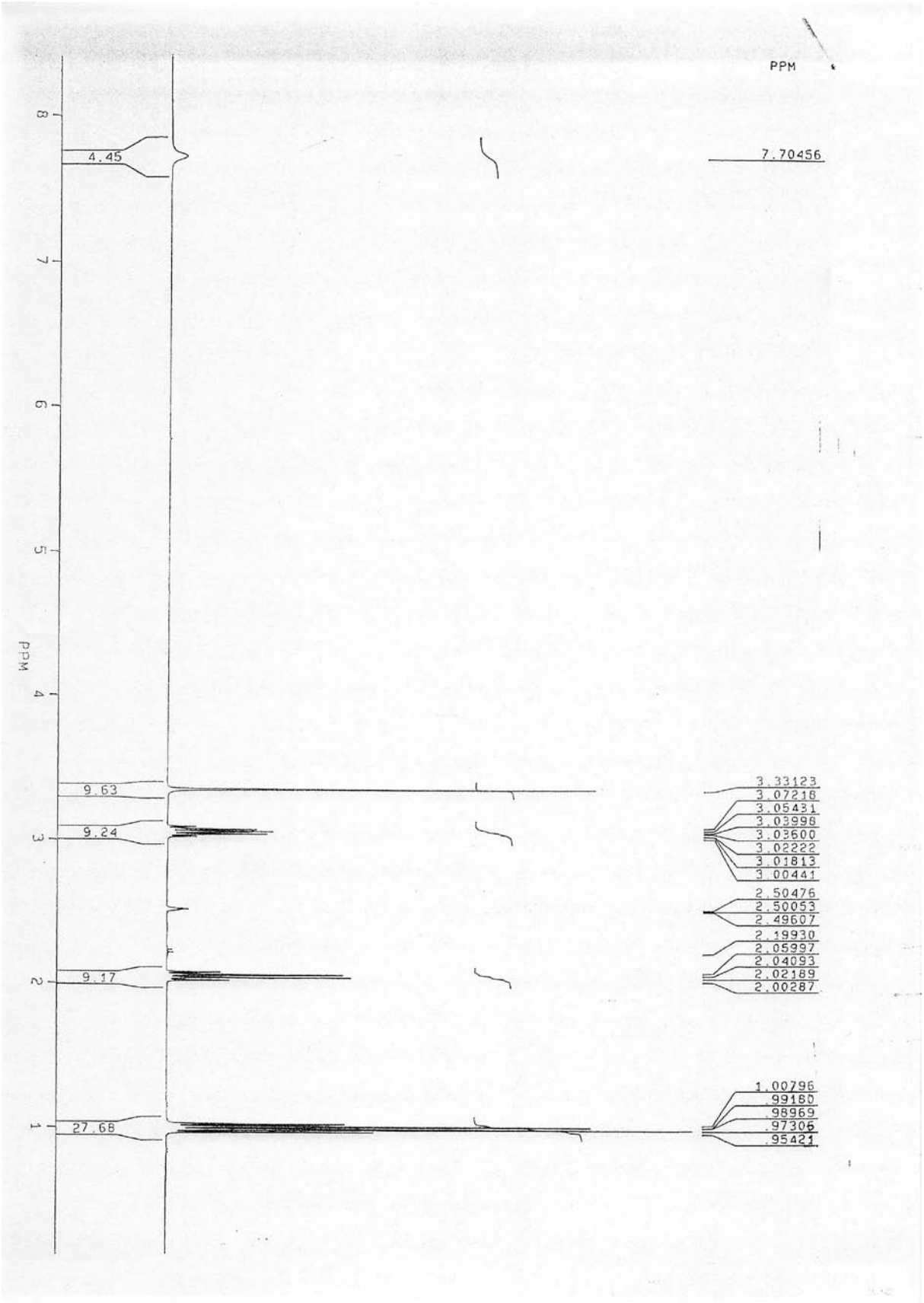
Compound **7**: D_2O



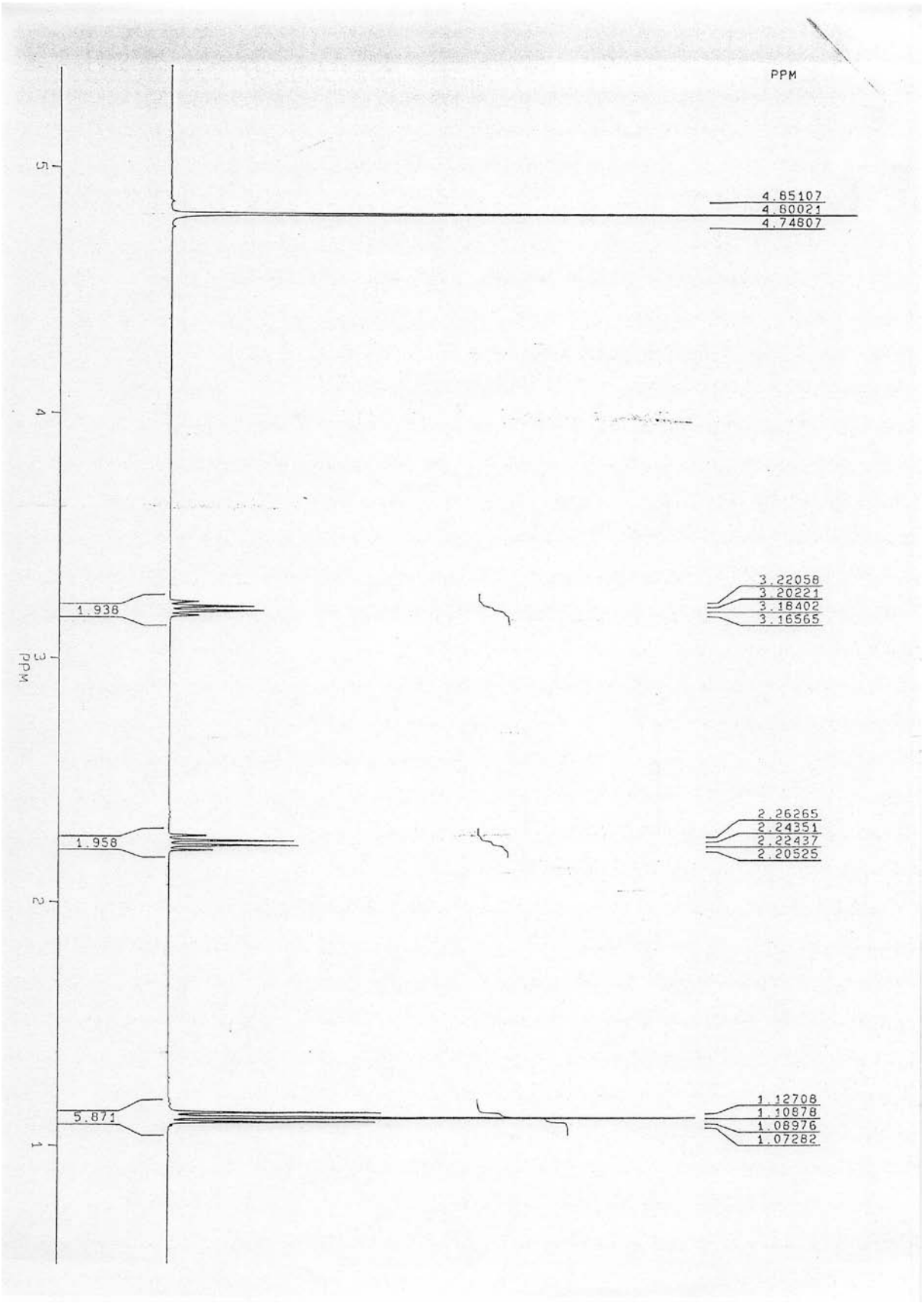
Compound **8**: $CDCl_3$



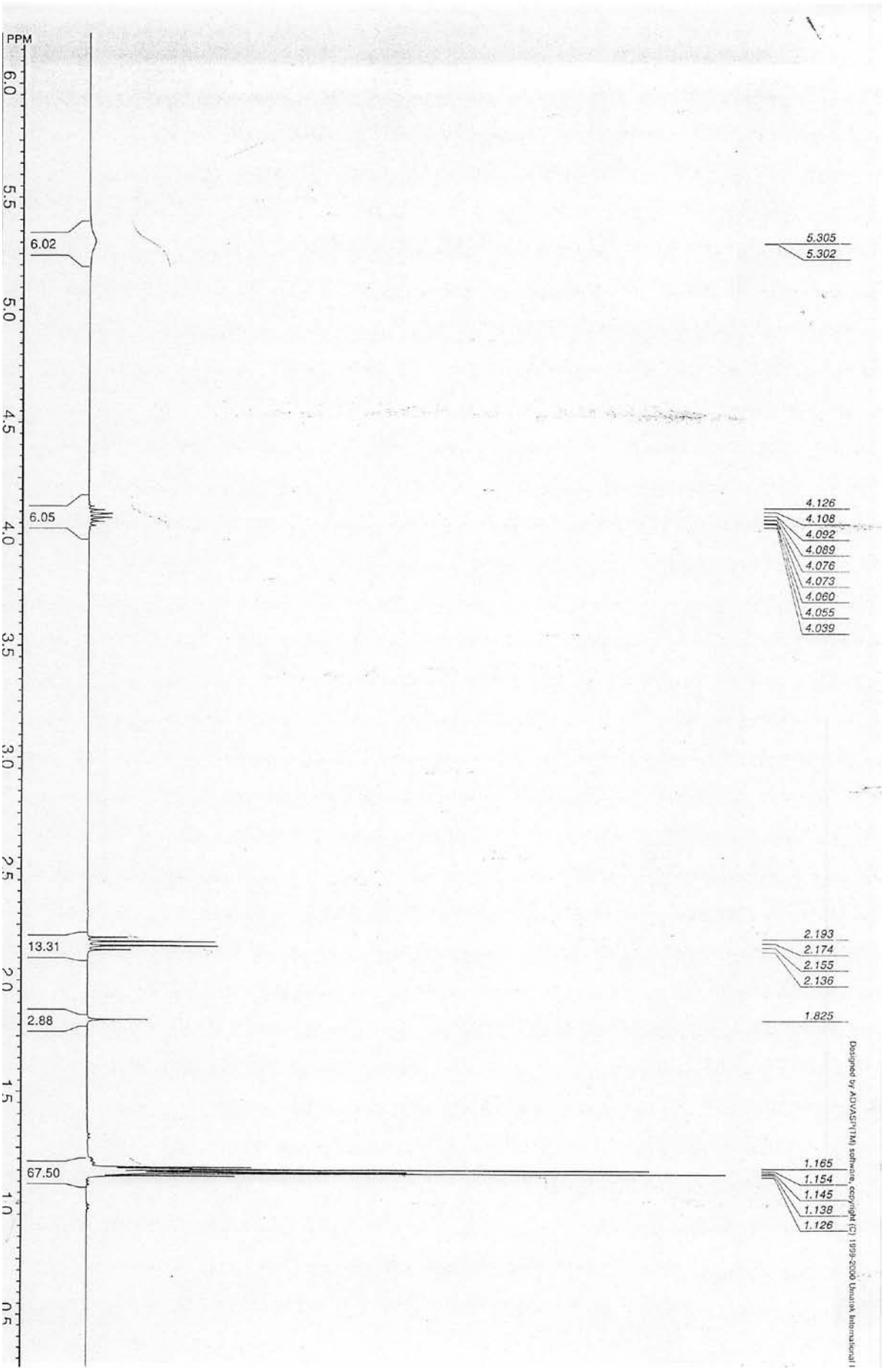
Compound **8**: DMSO-d_6



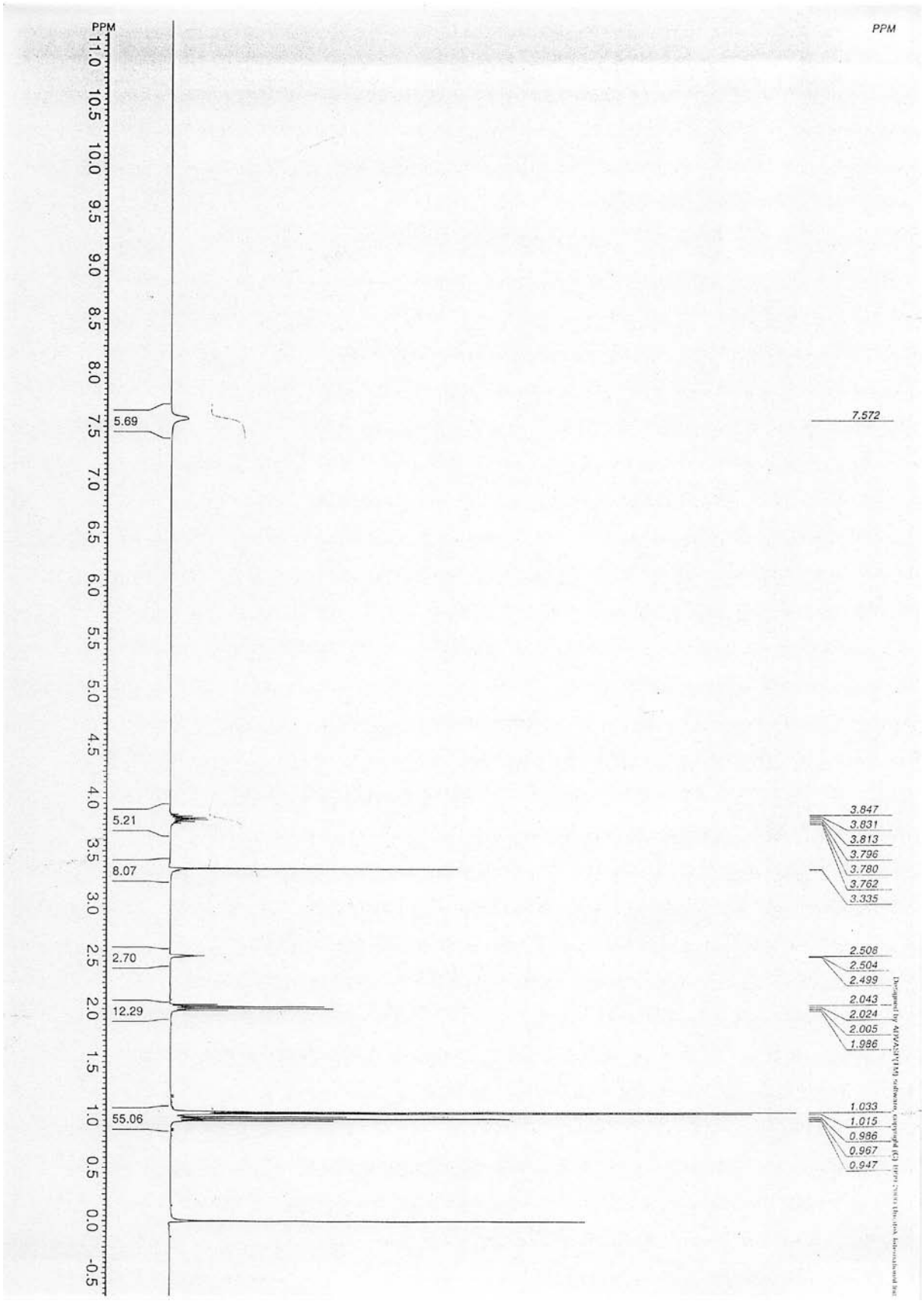
Compound **8**: D_2O



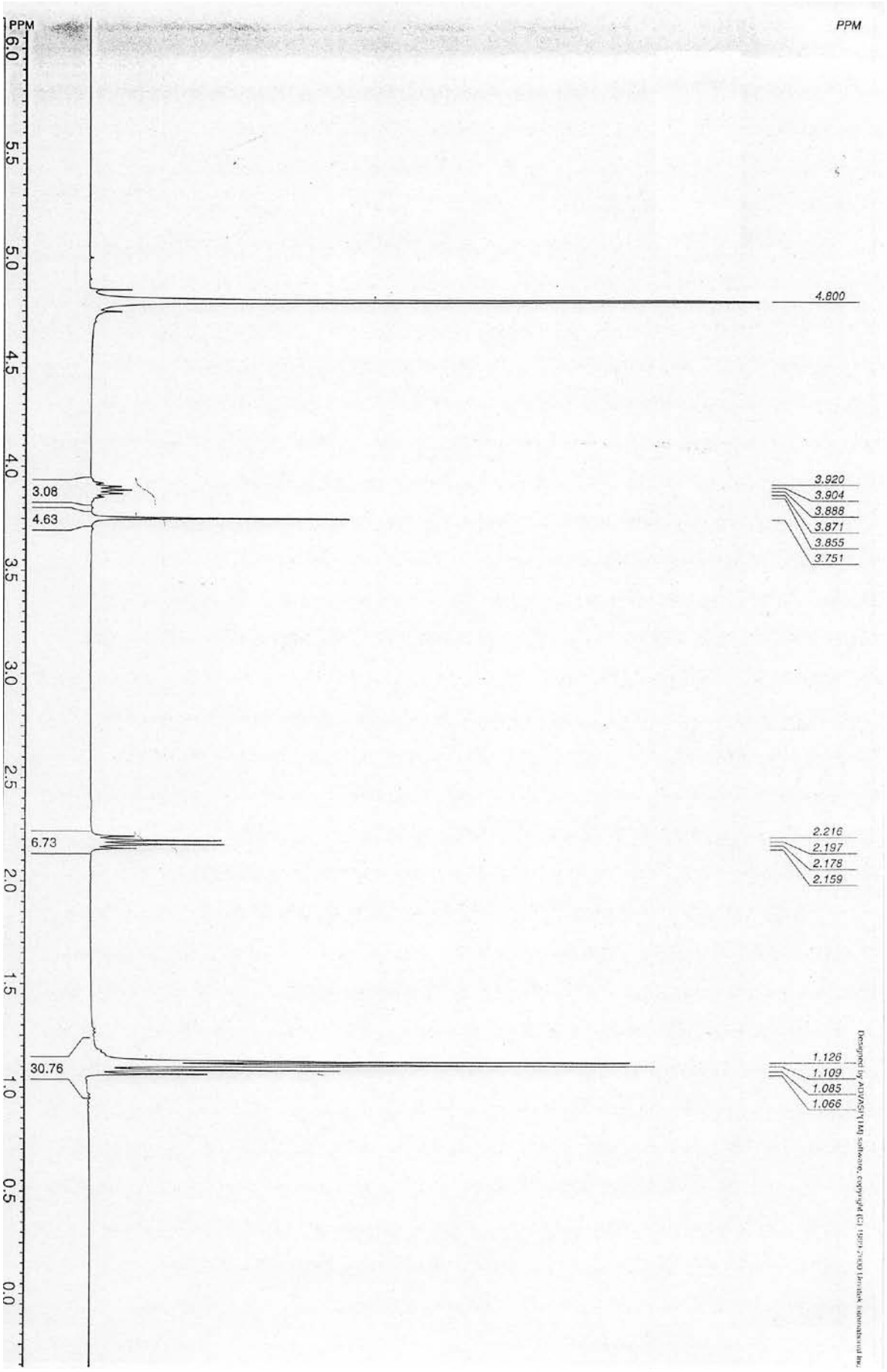
Compound **9**: $CDCl_3$



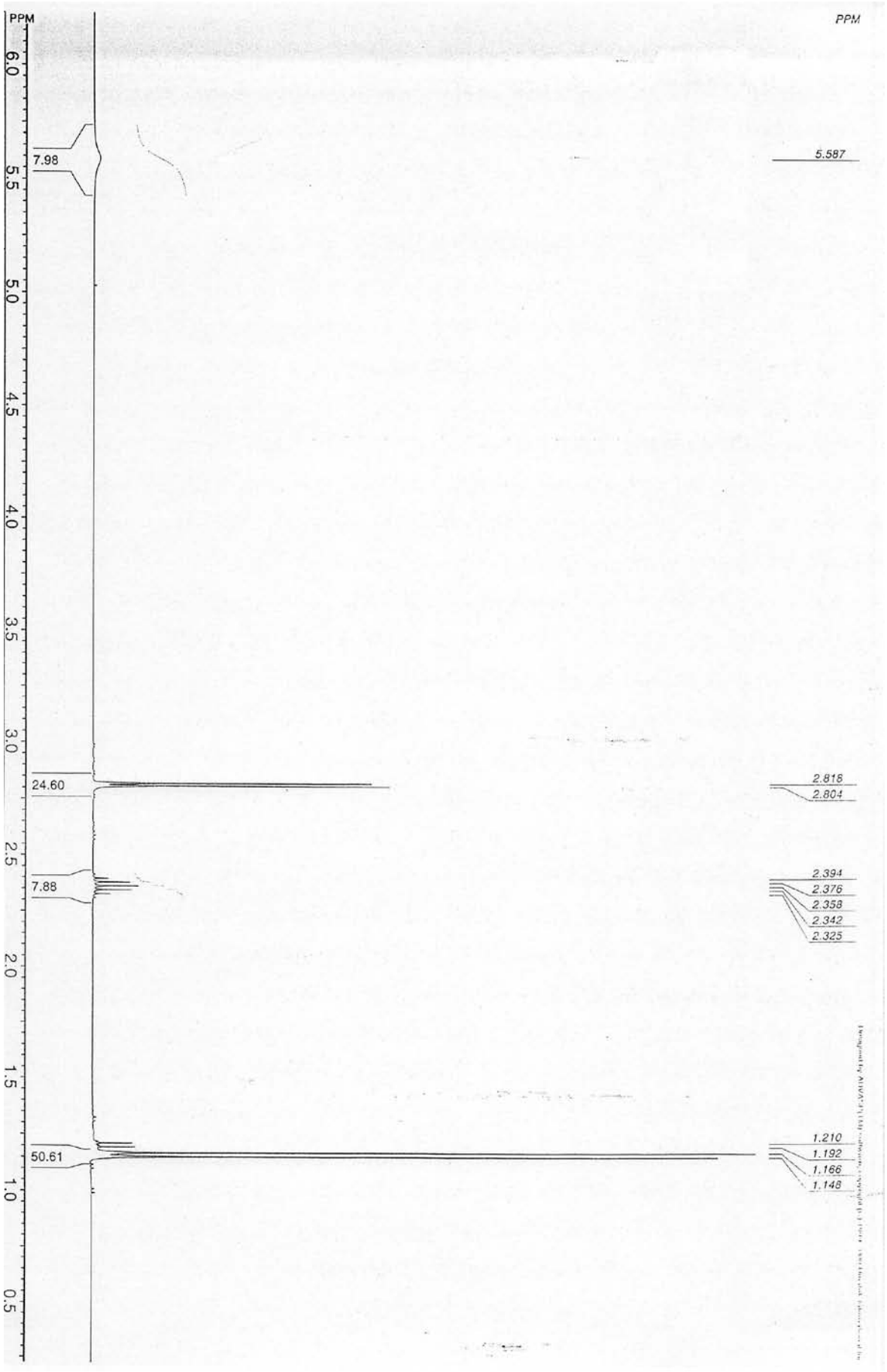
Compound **9**: DMSO-d_6



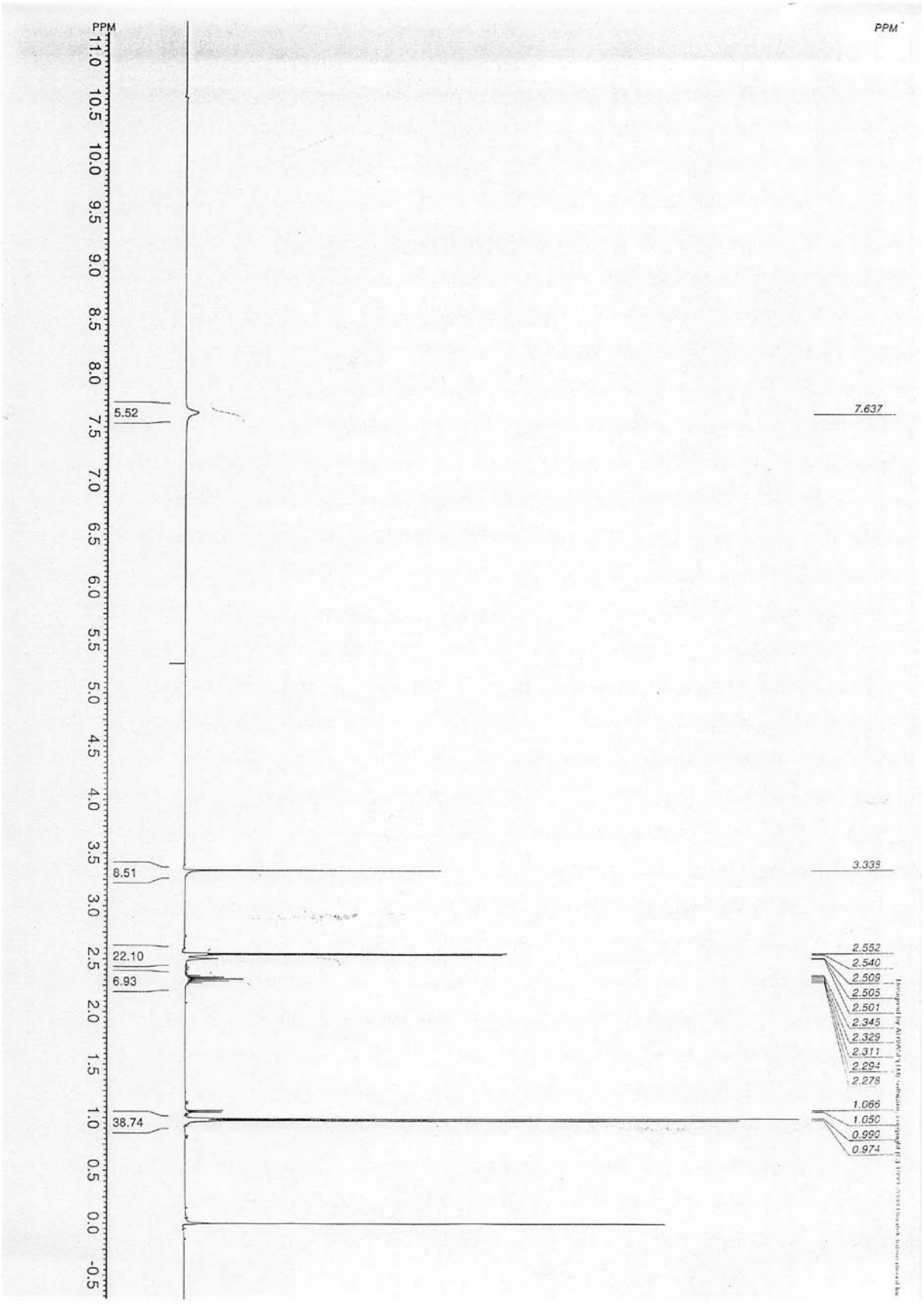
Compound **9**: D_2O



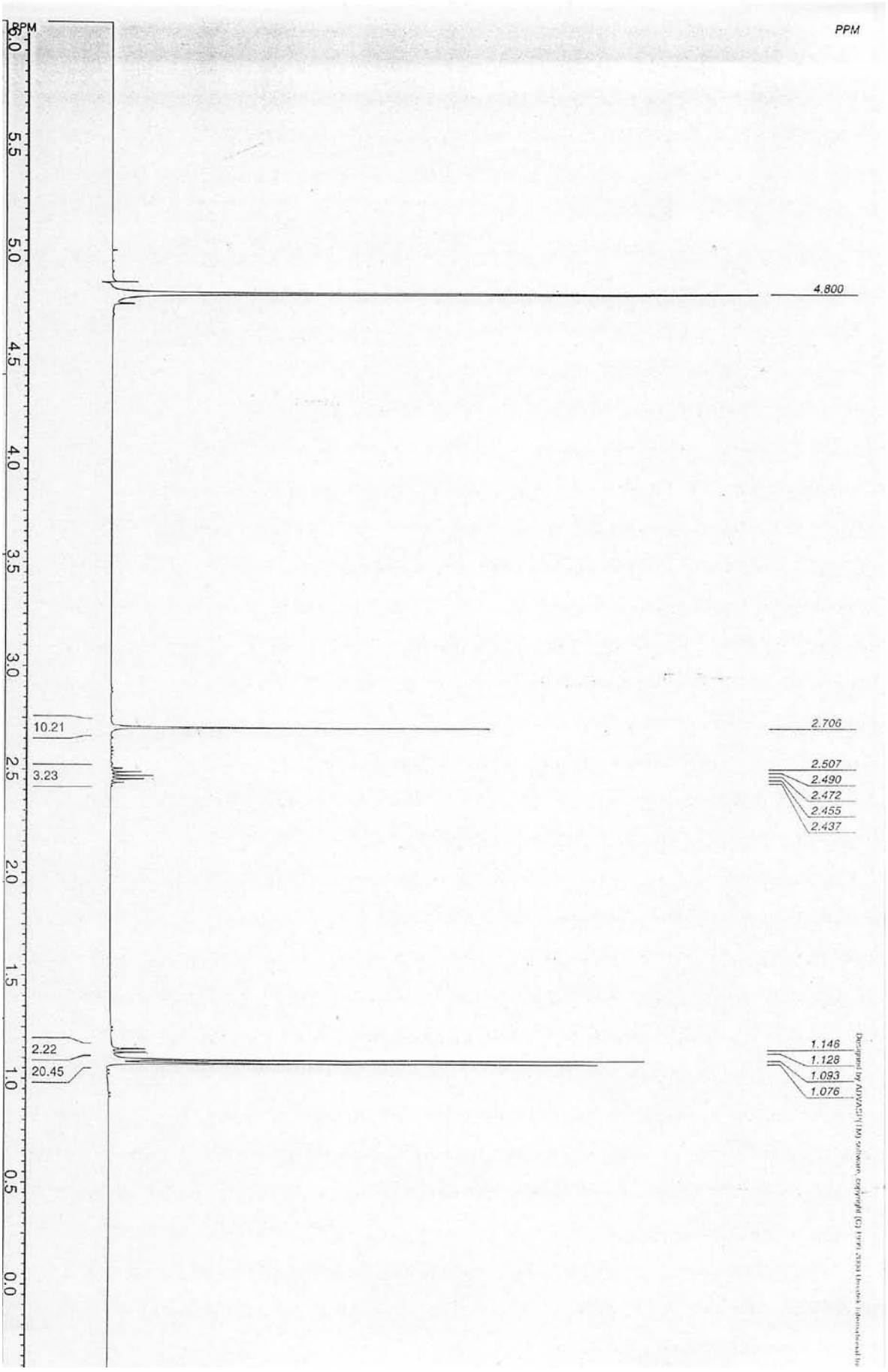
Compound **10**: $CDCl_3$



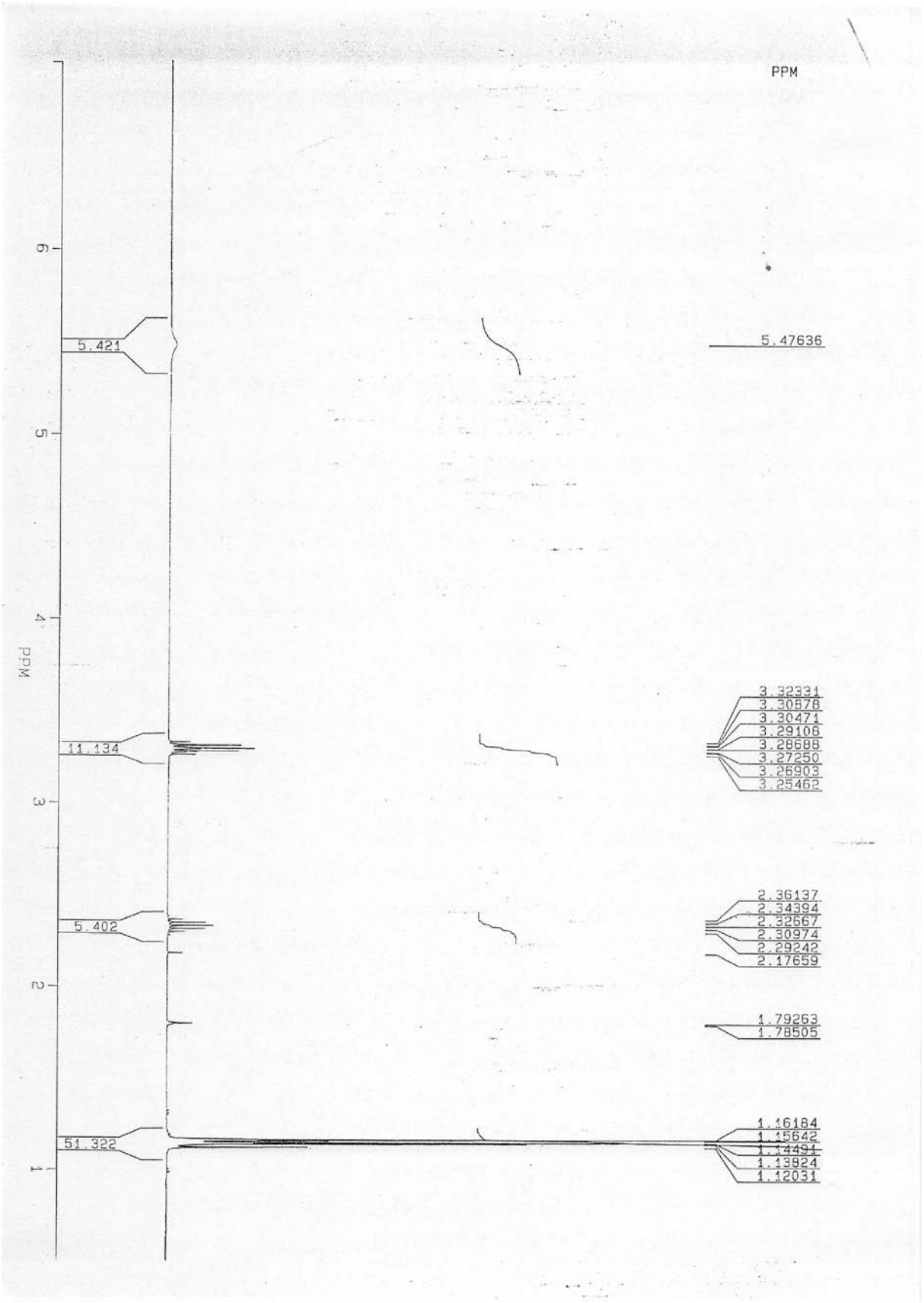
Compound **10**: DMSO-d_6



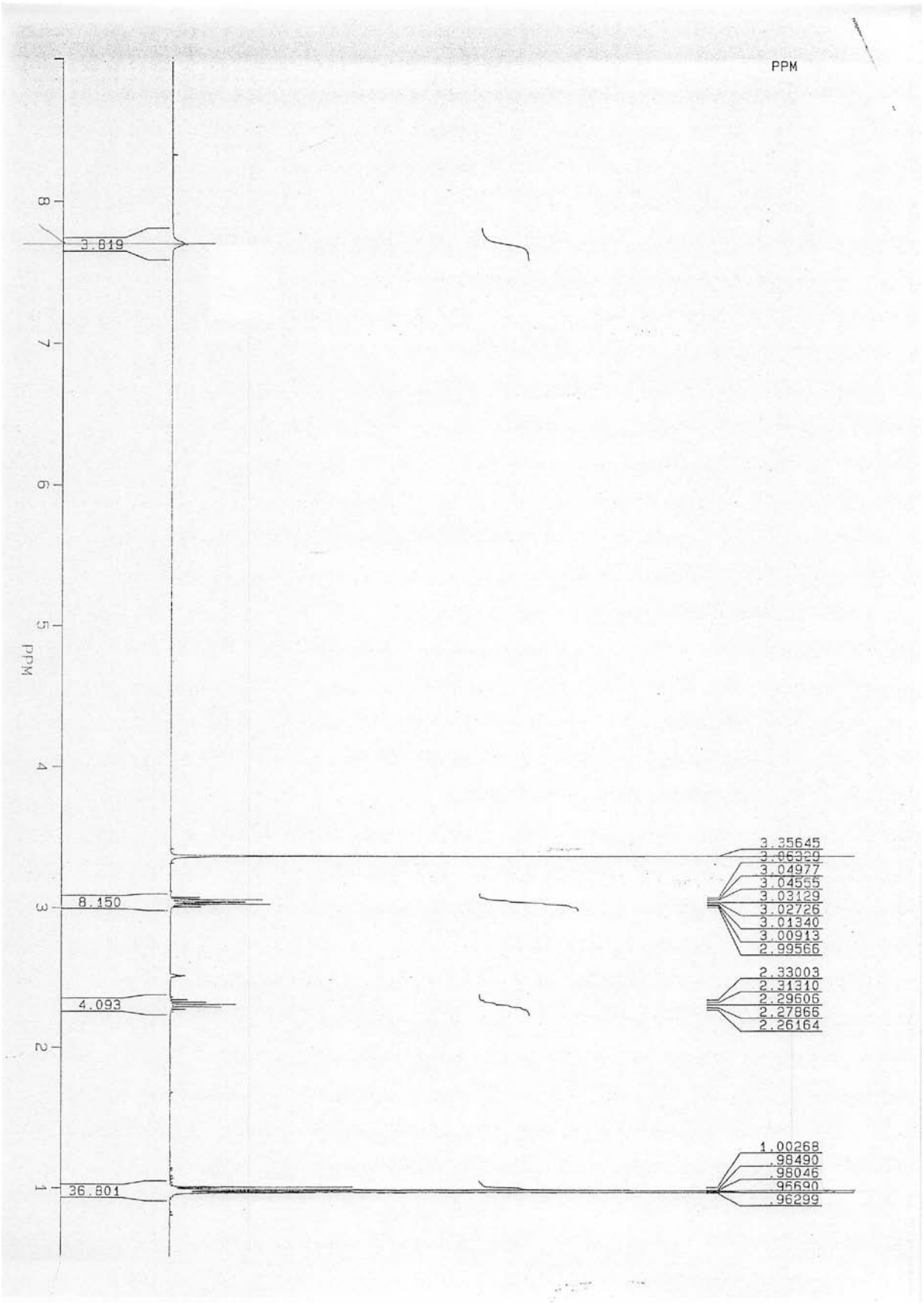
Compound **10**: D_2O



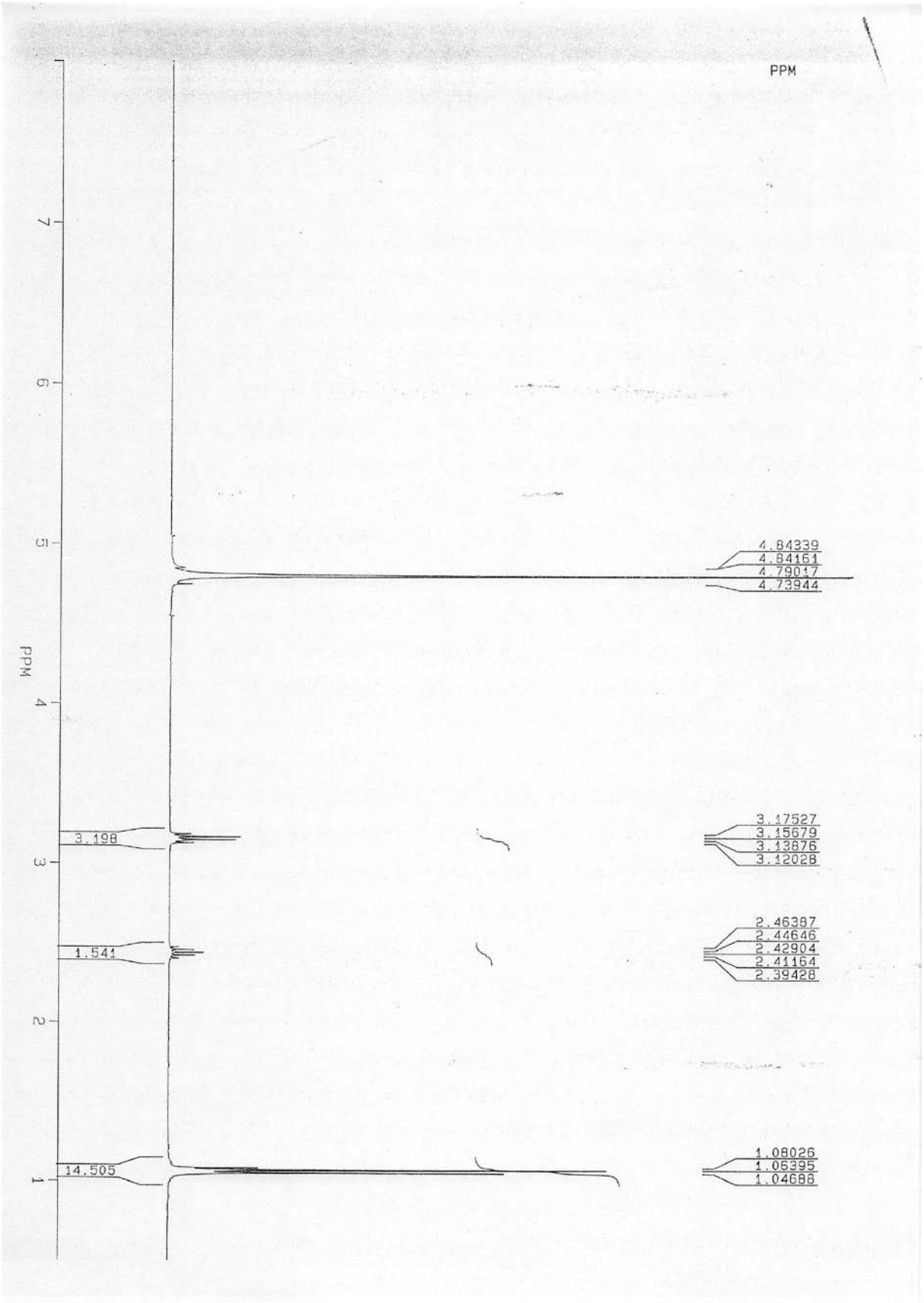
Compound **11**: $CDCl_3$



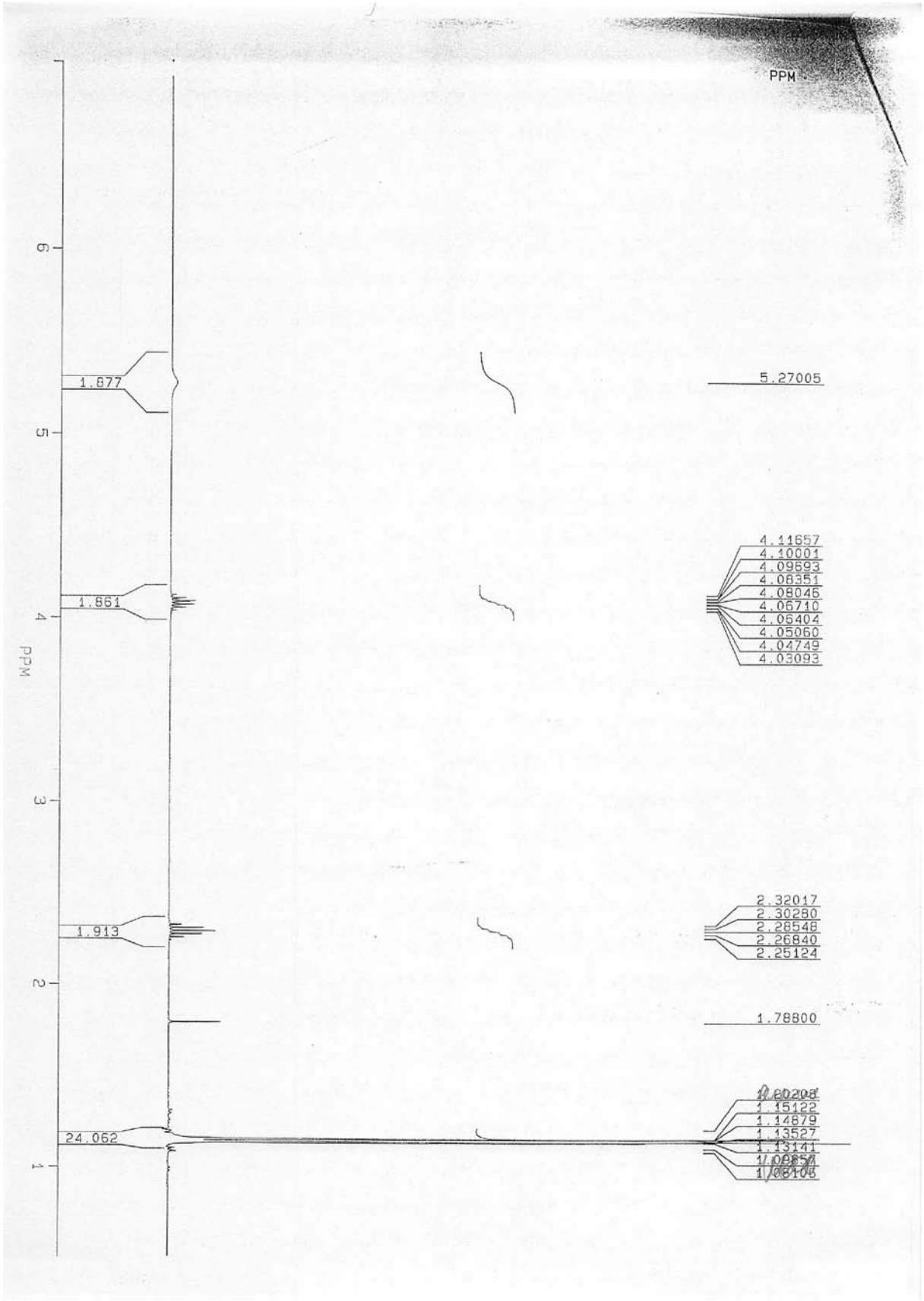
Compound **11**: DMSO-d_6



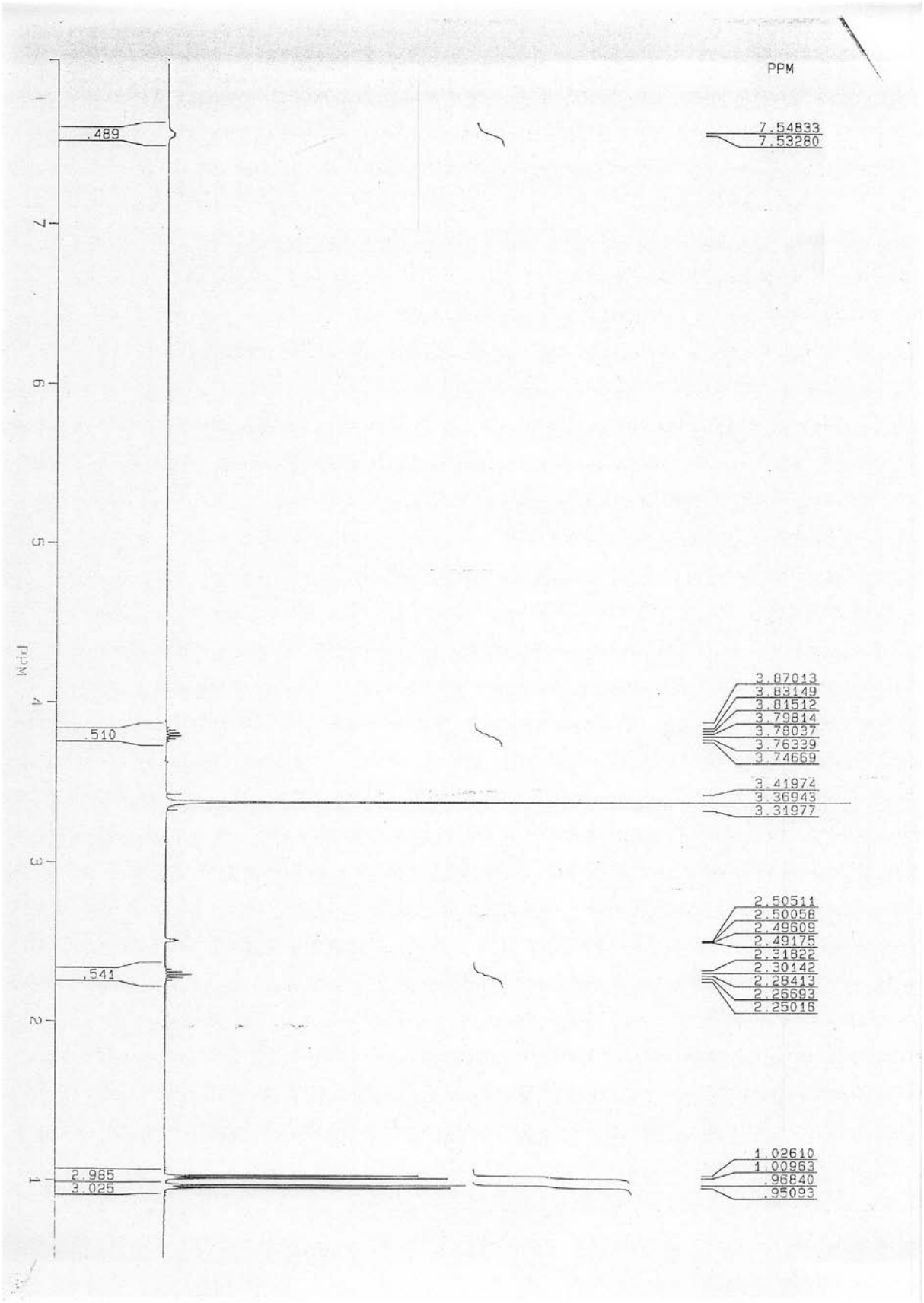
Compound **11**: D_2O



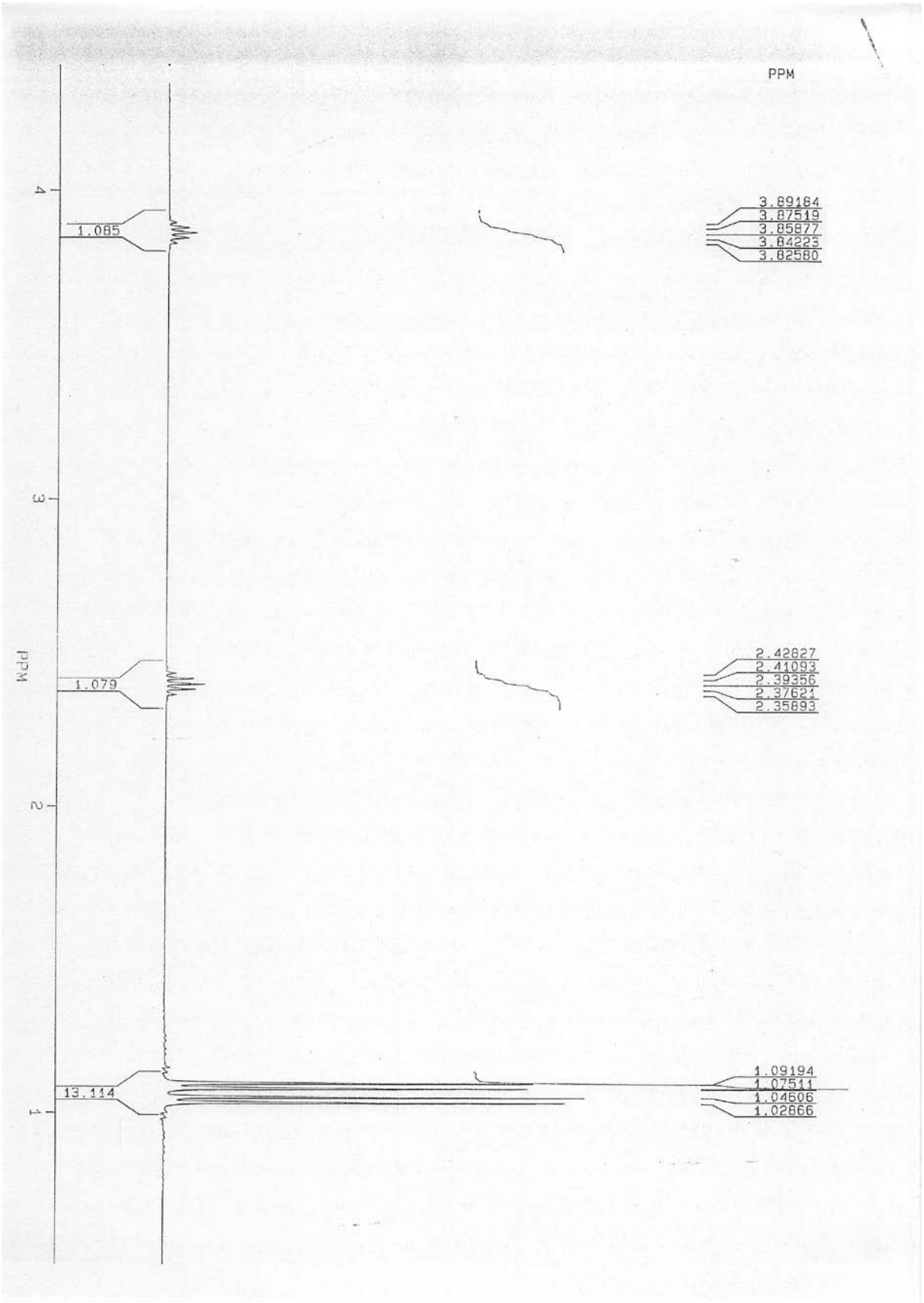
Compound **12**: $CDCl_3$



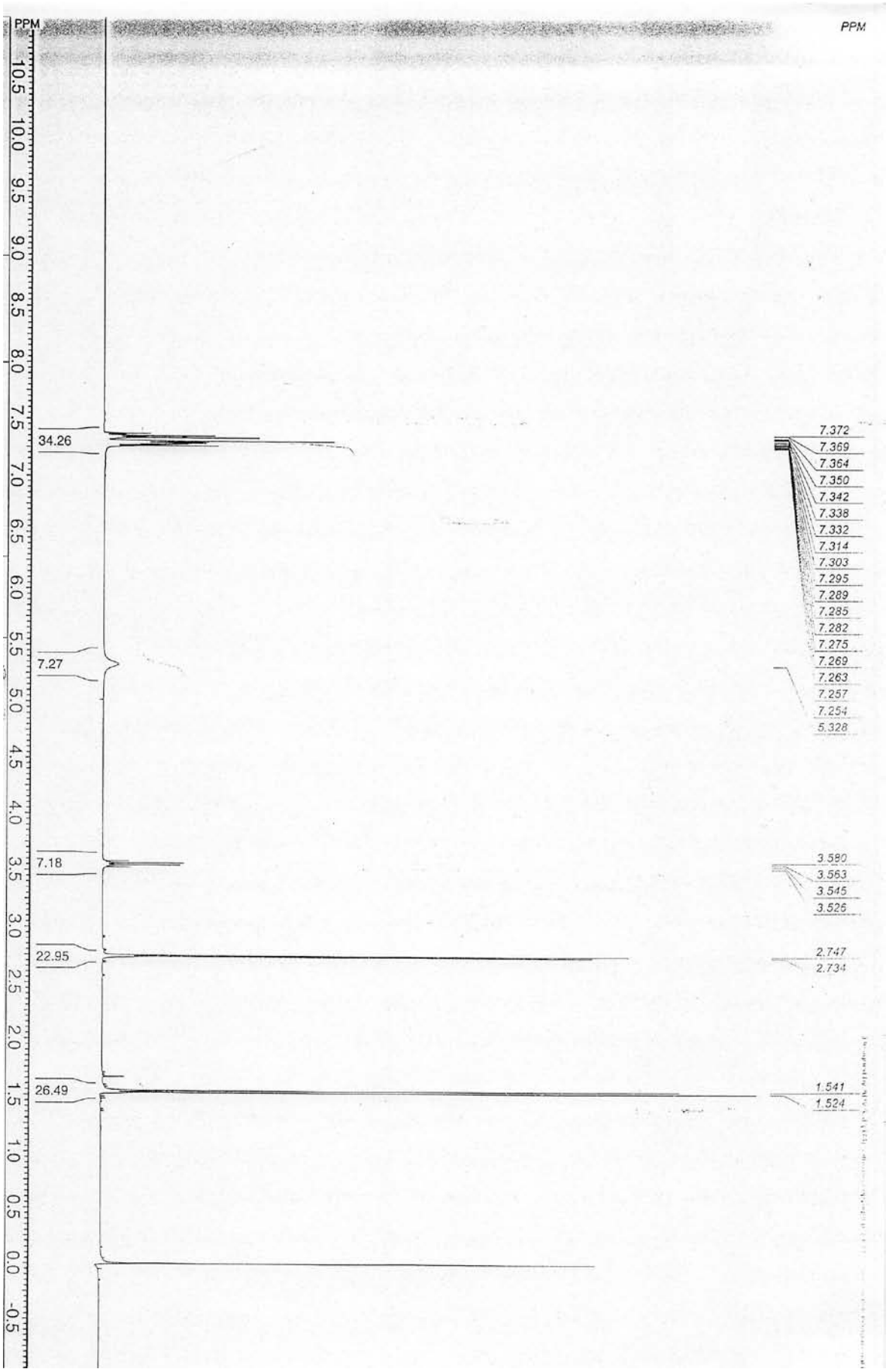
Compound **12**: DMSO-d_6



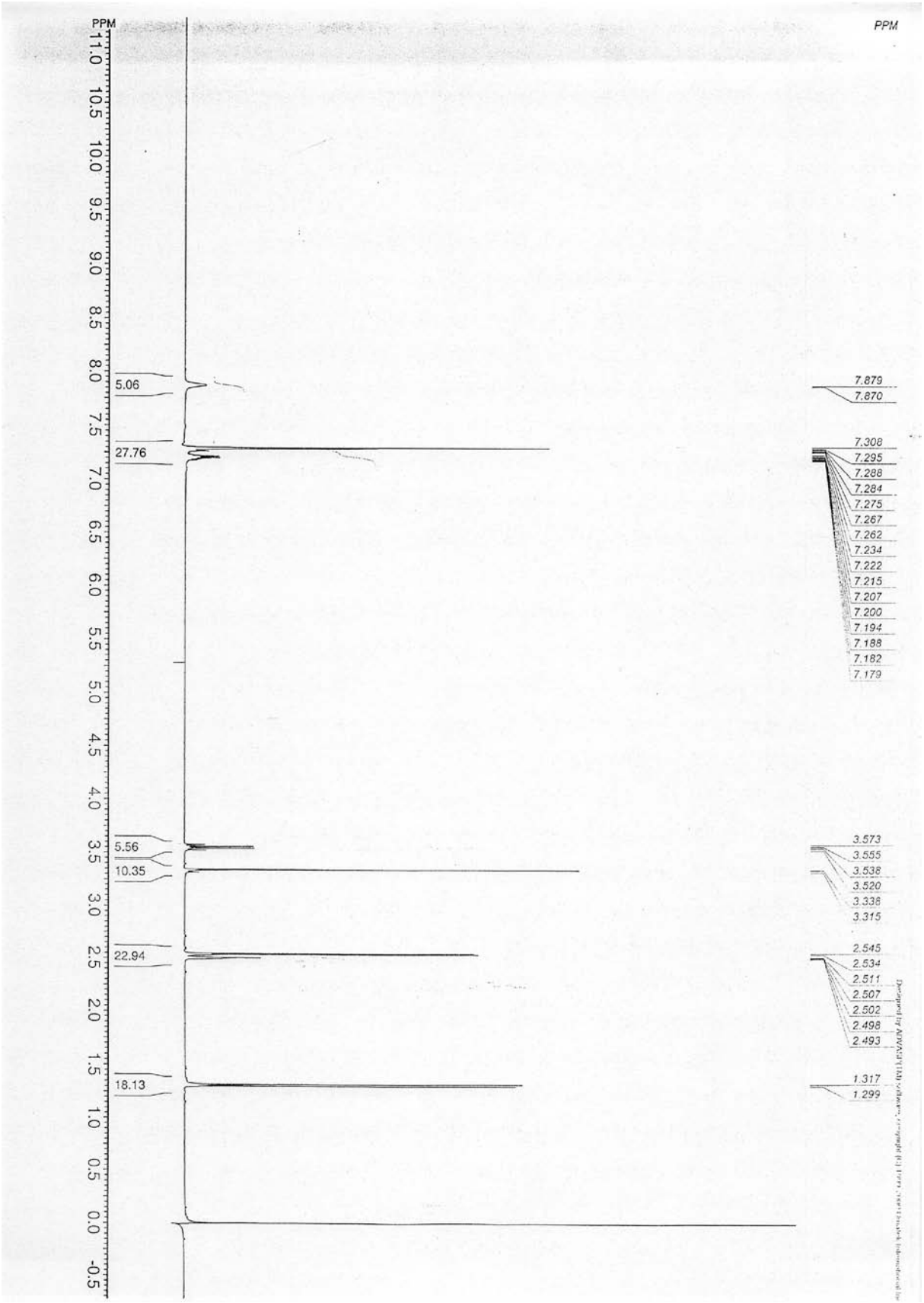
Compound **12**: D_2O



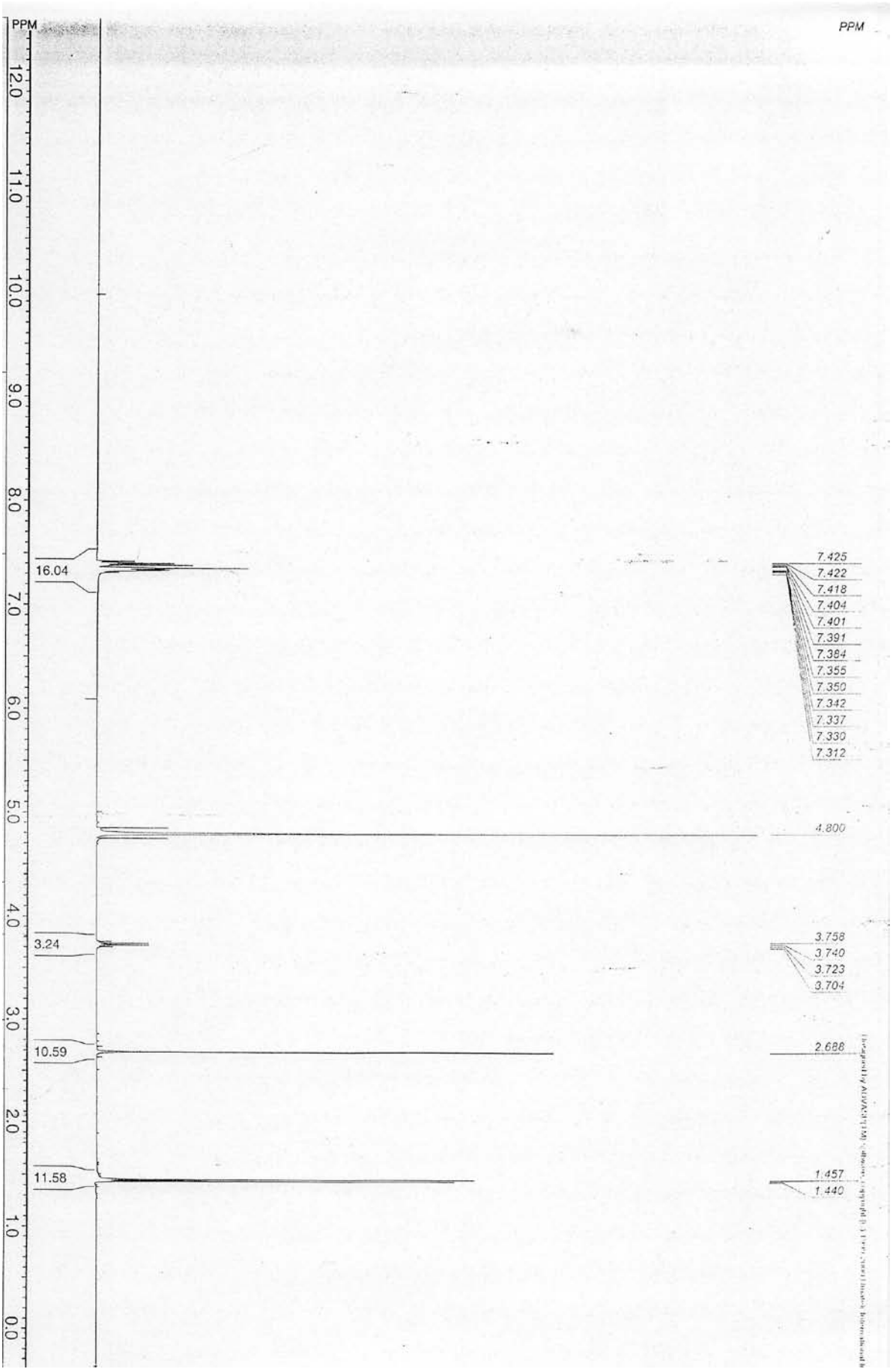
Compound **13**: $CDCl_3$



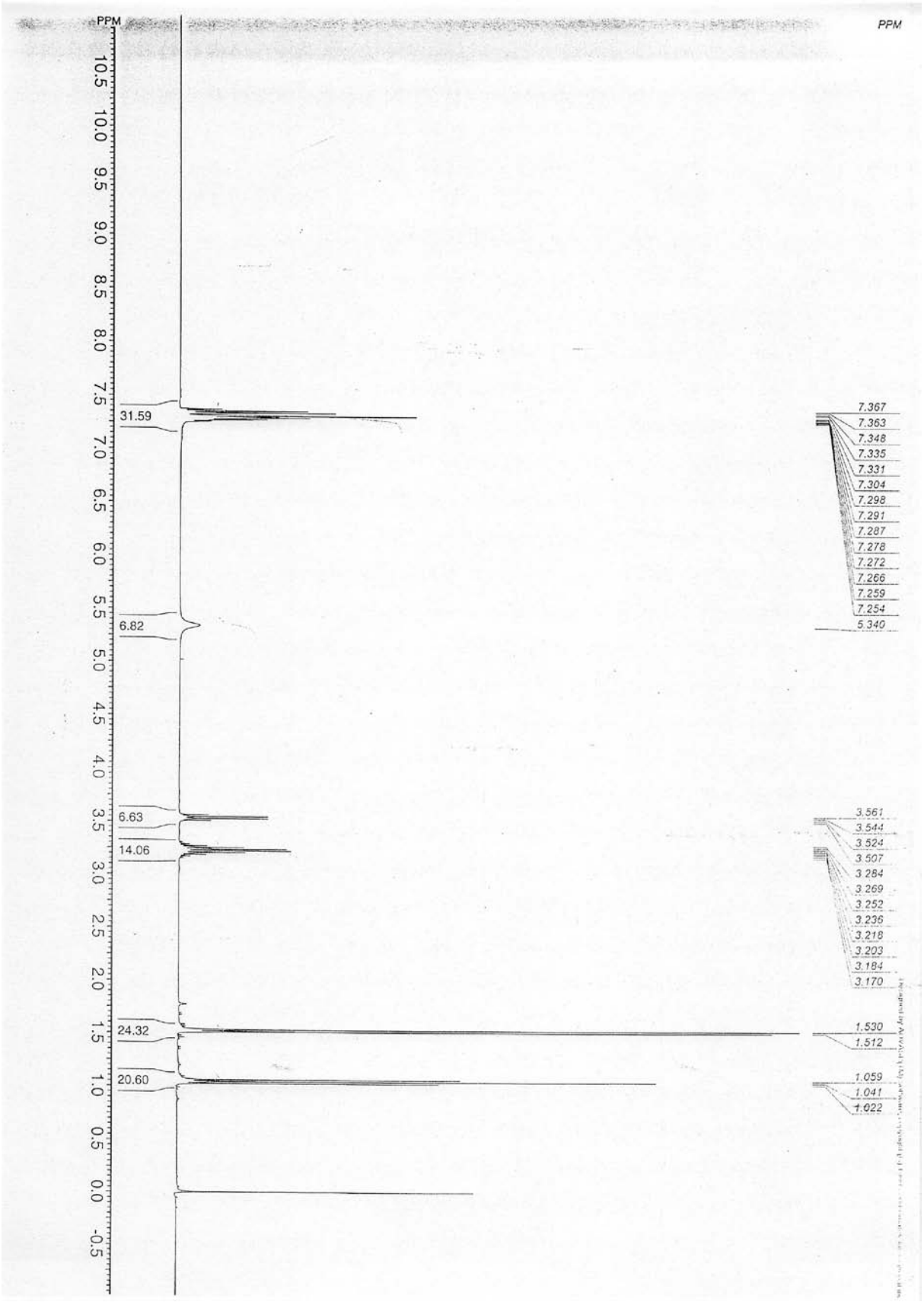
Compound **13**: DMSO-d_6



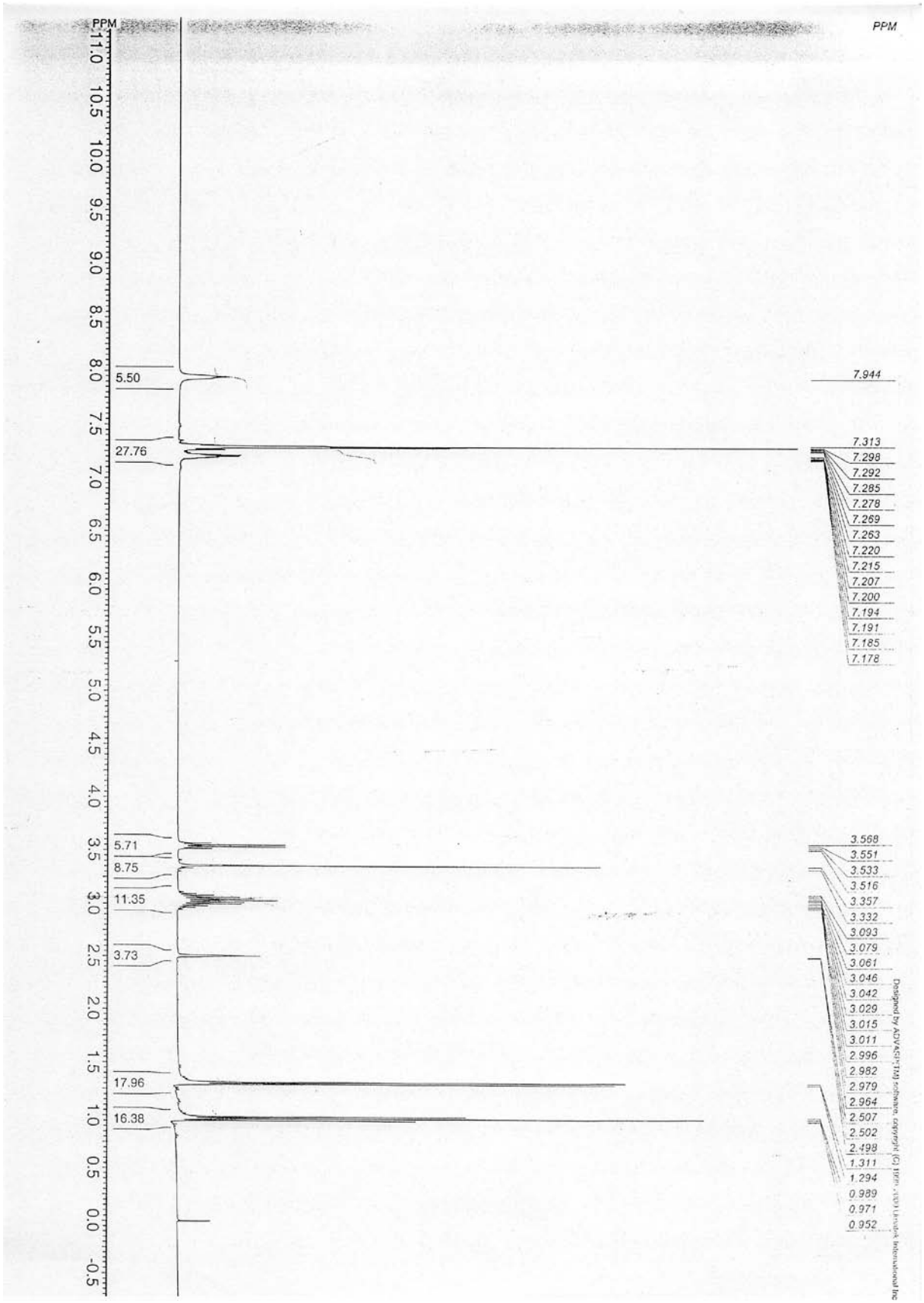
Compound **13**: D_2O



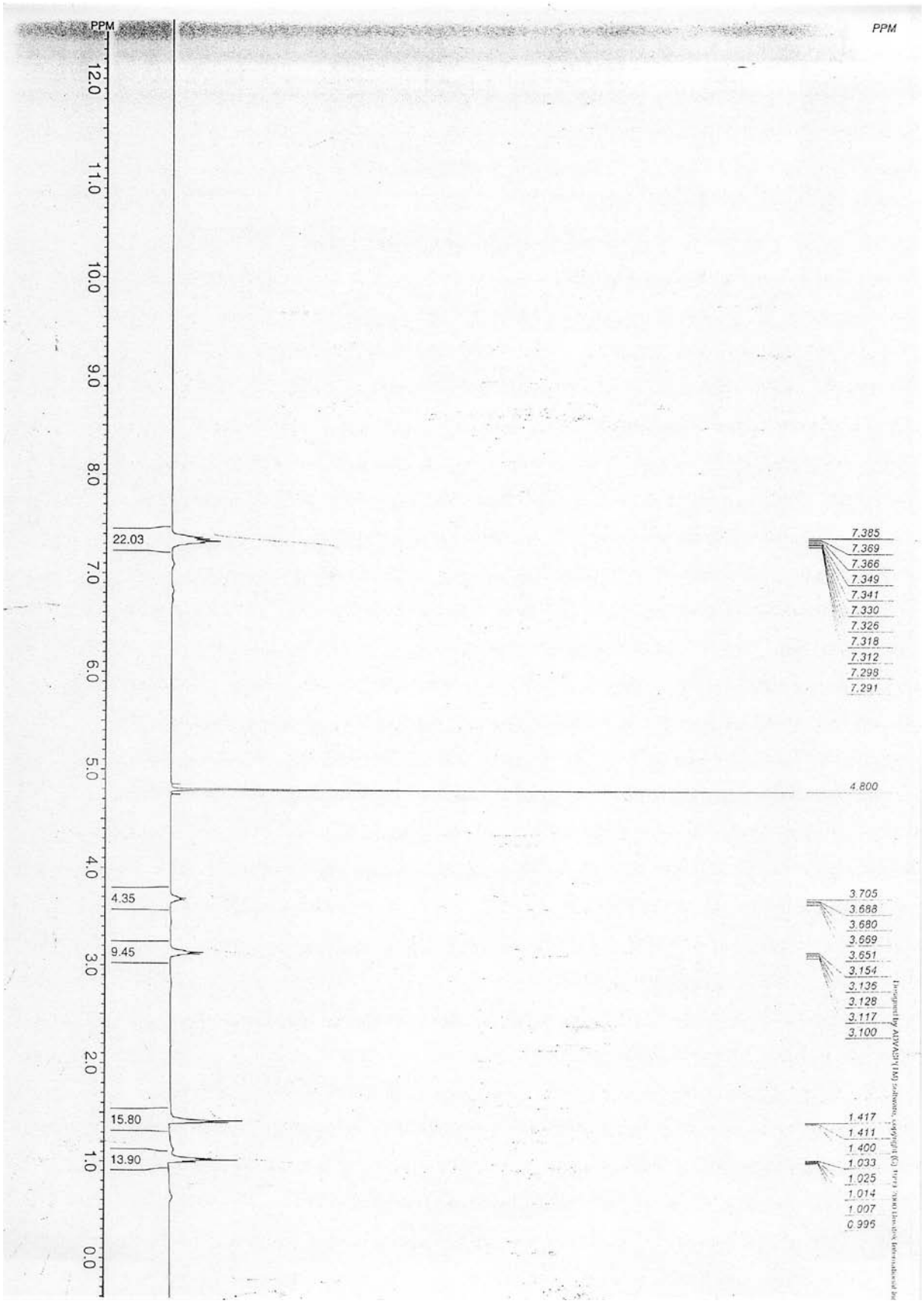
Compound **14**: $CDCl_3$



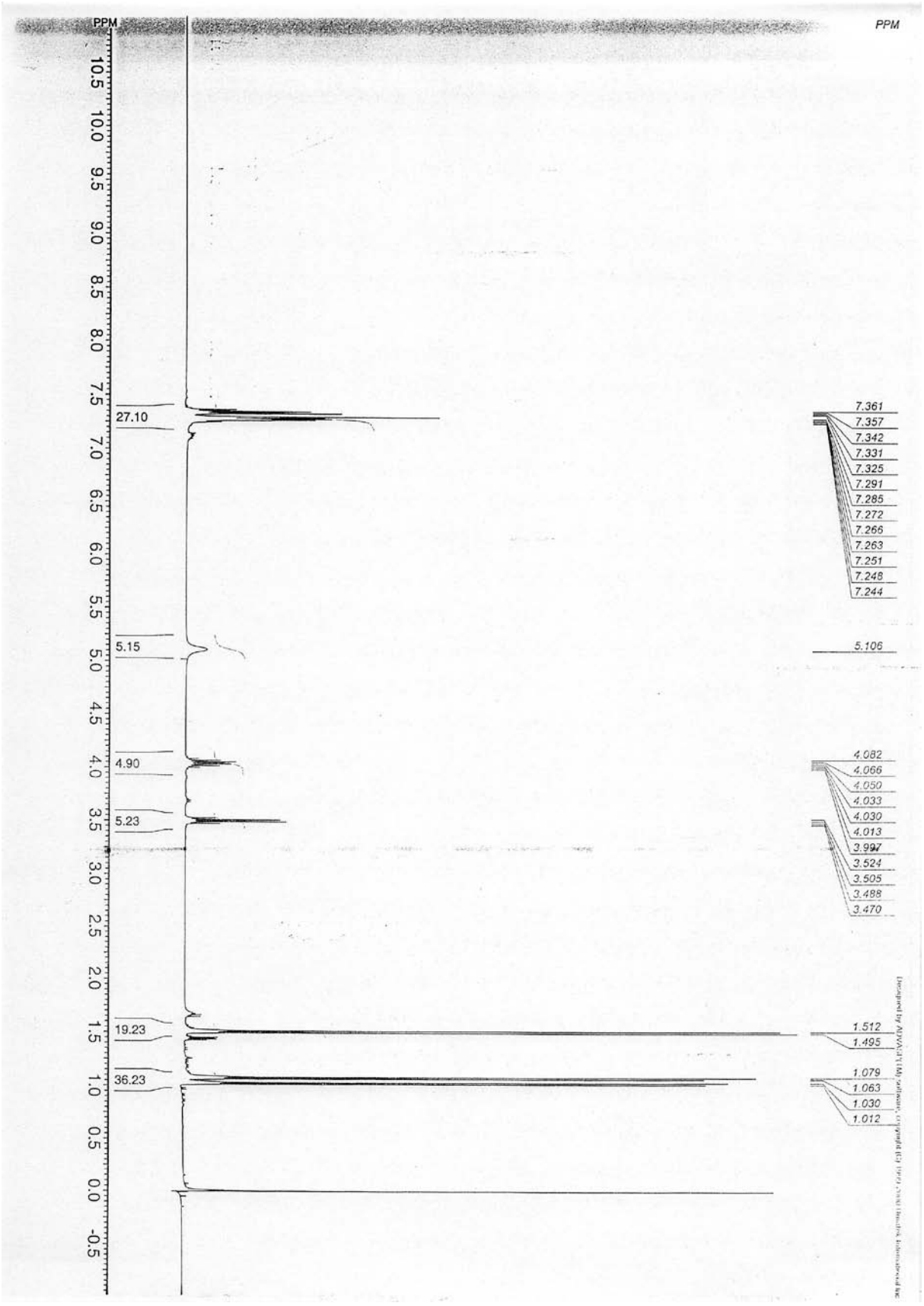
Compound **14**: DMSO-d_6



Compound **14**: D_2O



Compound **15**: $CDCl_3$



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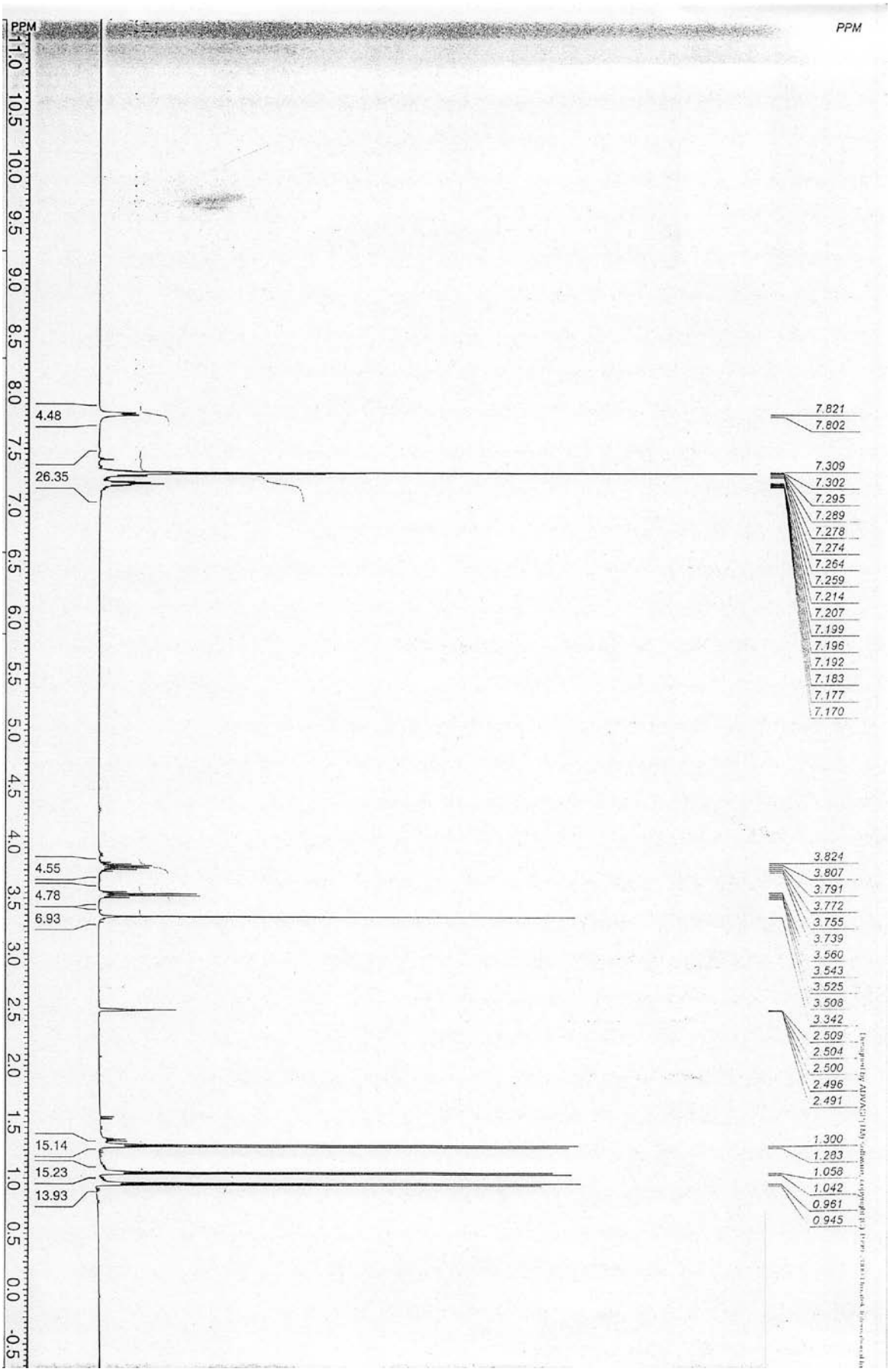

Compound **15**: D_2O