Supporting Information

Synthesis, optical resolution, absolute configuration, and osteogenic activity of *cis*-pterocarpans

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E-mail address: bringman@chemie.uni-wuerzburg.de (G. Bringmann).

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EXPERIMENTAL DATA

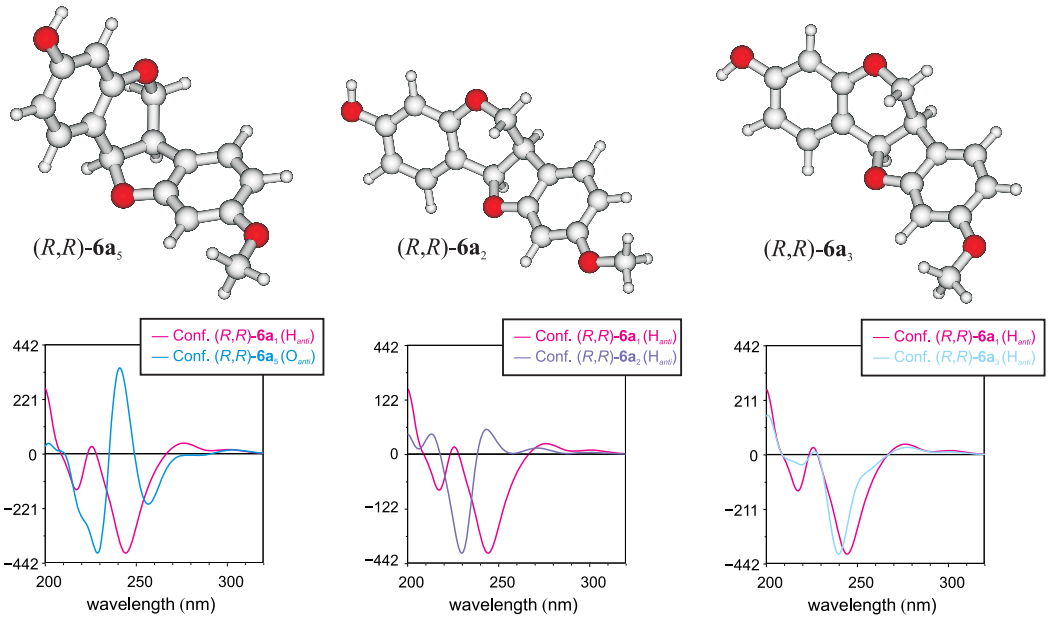

Figure S1. Analysis of the different conformations of the backbone (H_{anti} or O_{anti}), OMe and OH groups arrangements of pterocarpans and their impact on the CD effect in comparison to the one of the global minimum exemplarily shown for (6a*R*,11a*R*)-medicarpin.

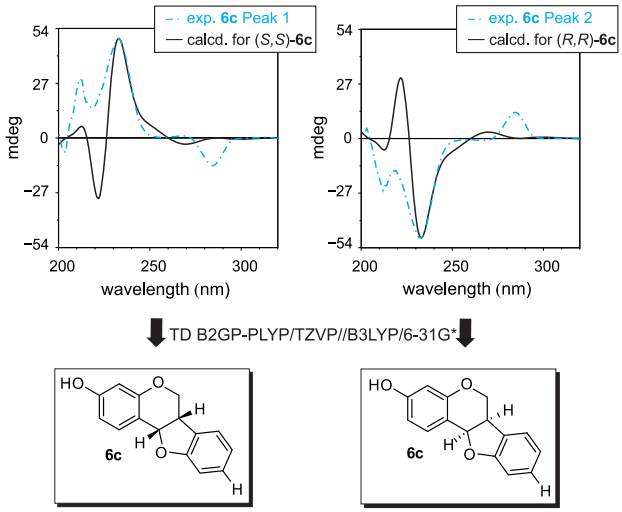

Figure S2. Comparison of the experimental CD spectra of both enantiomers of **6c** with the CD curves calculated for (6a*R*,11a*R*)-**6c** and (6a*S*,11a*S*)-**6c** using the TDB2GP-PLYP method.

HPLC Chromatograms

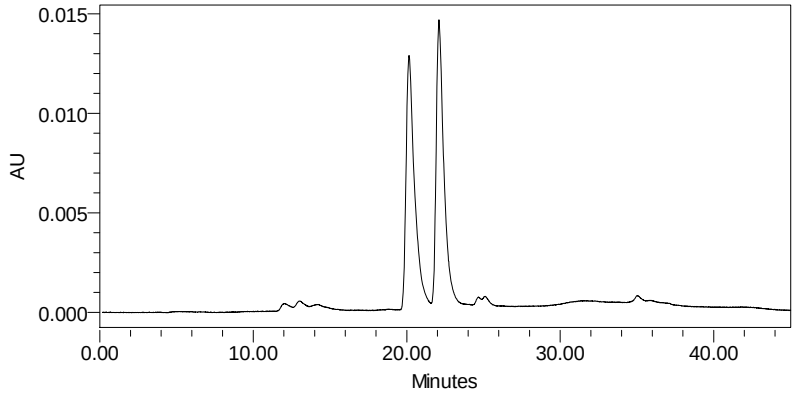

Table S1

S. No.	Name	Retention Time	Area	% Area	Height	Wavelength (nm)
1	Peak 1	20.153	512917	49.57	13255	286.5
2	Peak 2	22.103	521735	50.43	14970	286.5

Figure S3: Chromatogram of *rac*-**6a**

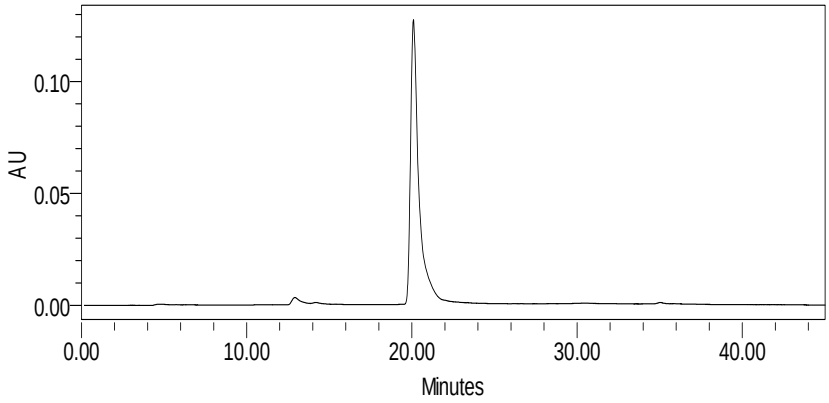

Table S2

S.No.	Name	Retention Time	Area	% Area	Height	Wavelength (nm)
1	Peak 1	20.098	4240178	100.00	120891	287.3

Figure S4: Chromatogram of (+)-**6a**

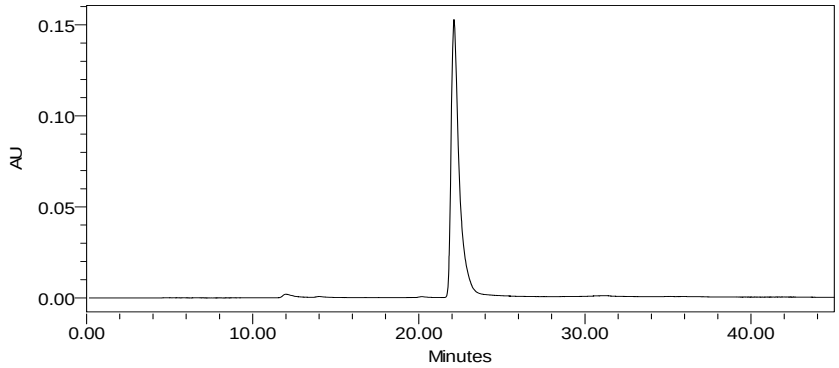

Table S3

S. No.	Name	Retention Time	Area	% Area	Height	Wavelength (nm)
1	Peak-1	20.165	24990	0.32	734	287.3
2	Peak-2	22.118	7753968	99.68	232707	287.3

Figure S5: Chromatogram of (–)-**6a**

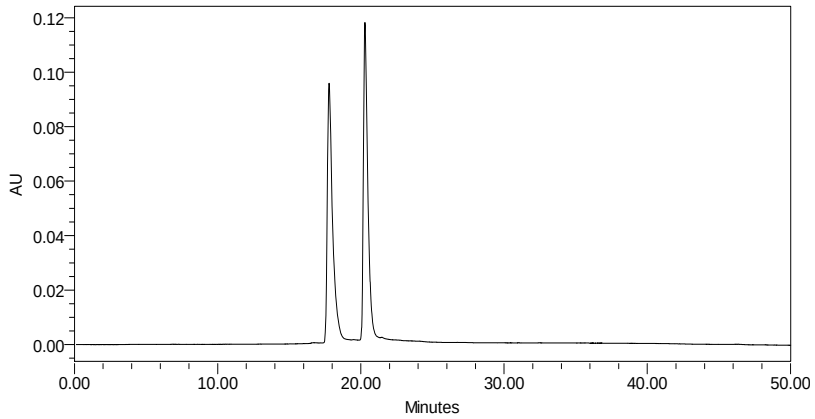

Table S4

S. No.	Name	Retention Time	Area	% Area	Height	Wavelength (nm)
1	Peak 1	17.779	2433035	49.55	95074	279
2	Peak 2	20.284	2476924	50.45	116445	279

Figure S6: Chromatogram of *rac*-**6c**

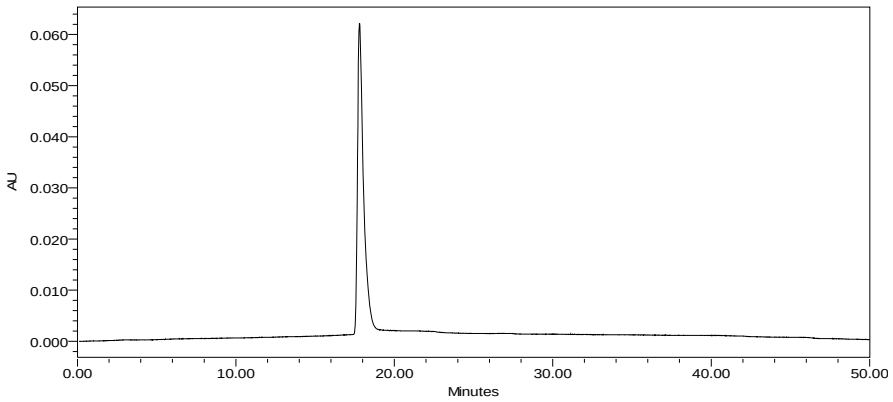

Table S5

S.No.	Name	Retention Time	Area	% Area	Height	Wavelength (nm)
1	Peak 1	17.804	1592979	100.00	60681	279

Figure S7: Chromatogram of (+)-**6c**

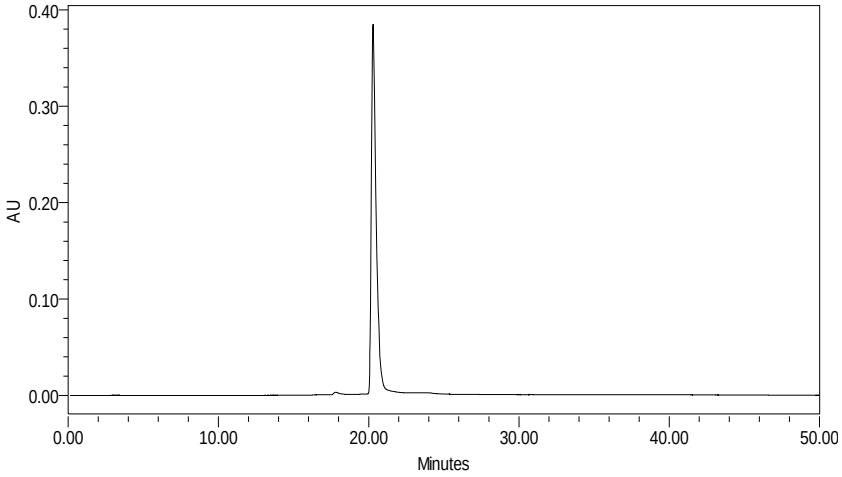

Table S6

S. No.	Name	Retention Time	Area	% Area	Height	Wavelength (nm)
1	Peak1	17.820	62379	0.74	2479	279
2	Peak2	20.288	8324170	99.26	382561	279

Figure S8:Chromatogram of (–)-**6c**

Instrument Method

Instrument Method (Analytical)

Instrument Method for compound 6a

Column used: ANALYTICAL PHENOMENIX (00G-4459-EOLUX5µ cellulose; 250X4.6mm)

S.No.	Time(min)	Flow	%water	%acetonitrile
1	0.0	0.50	50	50
2	7	0.50	40	60
3	10	0.50	20	80
4	12	0.50	10	90
5	25	0.50	10	90
6	30	0.50	20	80
7	35	0.50	40	60
8	40	0.50	50	50
9	50	0.50	50	50

Instrument Method for compound 6c

Column used: PHENOMENIX (00G-4459-EOLUX5µ cellulose; 250X4.6mm)

S.No.	Time(min)	Flow	%water	%acetonitrile
1	0.0	0.5	30	70
2	9	0.5	30	70
3	11	0.5	10	90
4	20	0.5	10	90
5	30	0.5	30	70
6	40	0.5	30	70
7	50	0.5	30	70

Instrument Method (Preparative)

Instrument Method for compound 6a

Column used: PHENOMENIX (005-4459-PO-RXLUX5µ Cellulose-1; 250X21mm)

S.No.	Time(min)	Flow(ml/min)	%water	%acetonitrile
1	0.01	5	50	50
2	0.02	5	50	50
3	10	5	40	60
4	25	5	20	80
5	35	5	15	85
6	45	5	15	85
7	50	5	50	50
8	60	0.0	50	50

Instrument Method for compound 6c

Column used: PHENOMENIX (005-4459-PO-RXLUX5µ Cellulose-1; 250X21mm)

S.No.	Time(min)	Flow(ml/min)	%water	%acetonitrile
1	0.01	6	45	55
2	.01	6	45	55
3	15	6	40	60
4	20	6	15	85
5	30	6	15	85
6	40	6	10	90
7	50	0.0	45	55

Supplementary Figures:

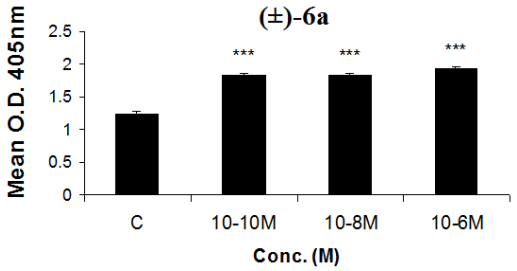

Figure S9. ALP activity of (±)-**6a** in rat calvarial derived osteoblast cells.

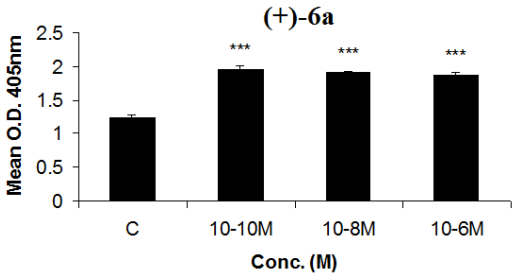

Figure S10. ALP activity of (+)-**6a** in rat calvarial derived osteoblast cells.

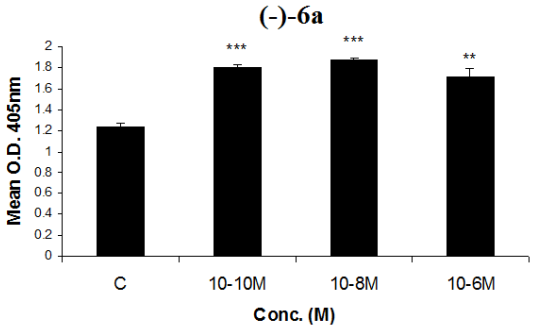

Figure S11. ALP activity of (–)-**6a** in rat calvarial derived osteoblast cells.

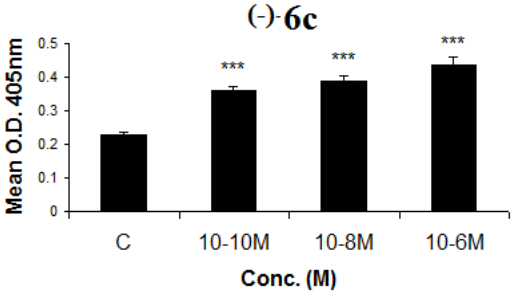

Figure S12. ALP activity in rat calvarial derived osteoblast cells ((–)-**6c**).

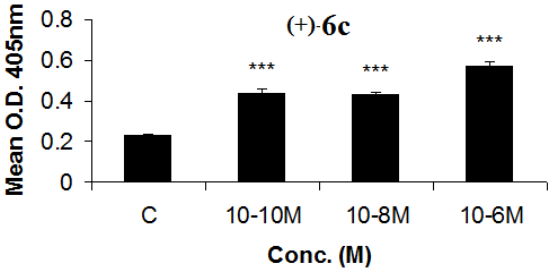

Figure S13. ALP activity in rat calvarial derived osteoblast cells ((+)-**6c**).

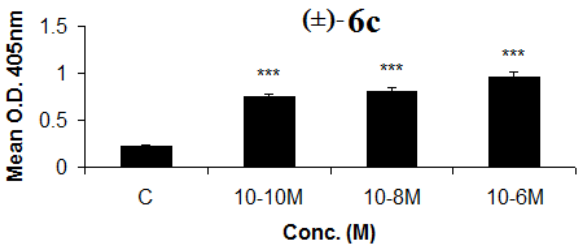

Figure S14. ALP activity in rat calvarial derived osteoblast cells ((±)-**6c**).

NMR spectra of synthesized compounds

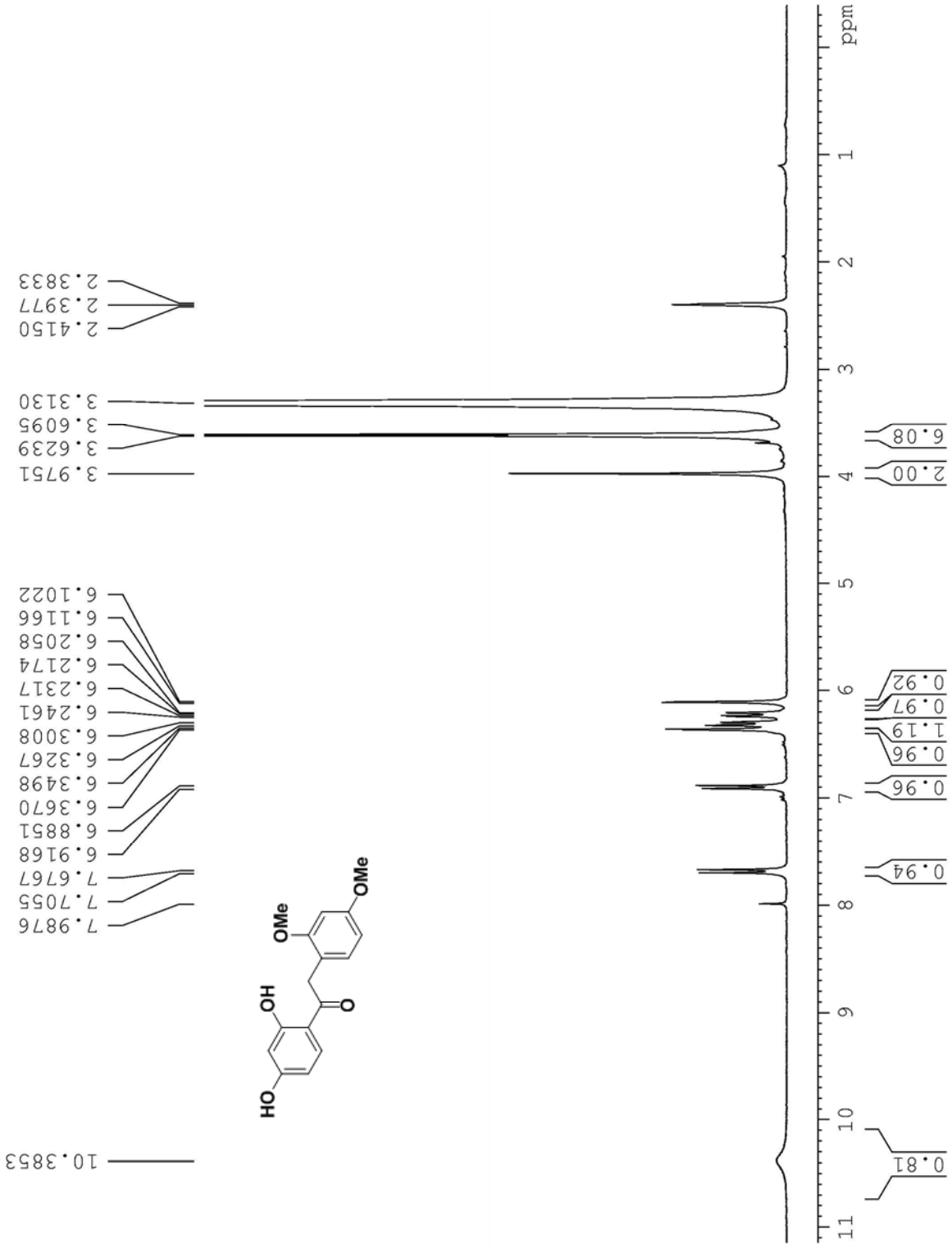

Figure S15. ^{1}H NMR spectrum of **3a** in $CDCl_3$ + DMSO-d_6

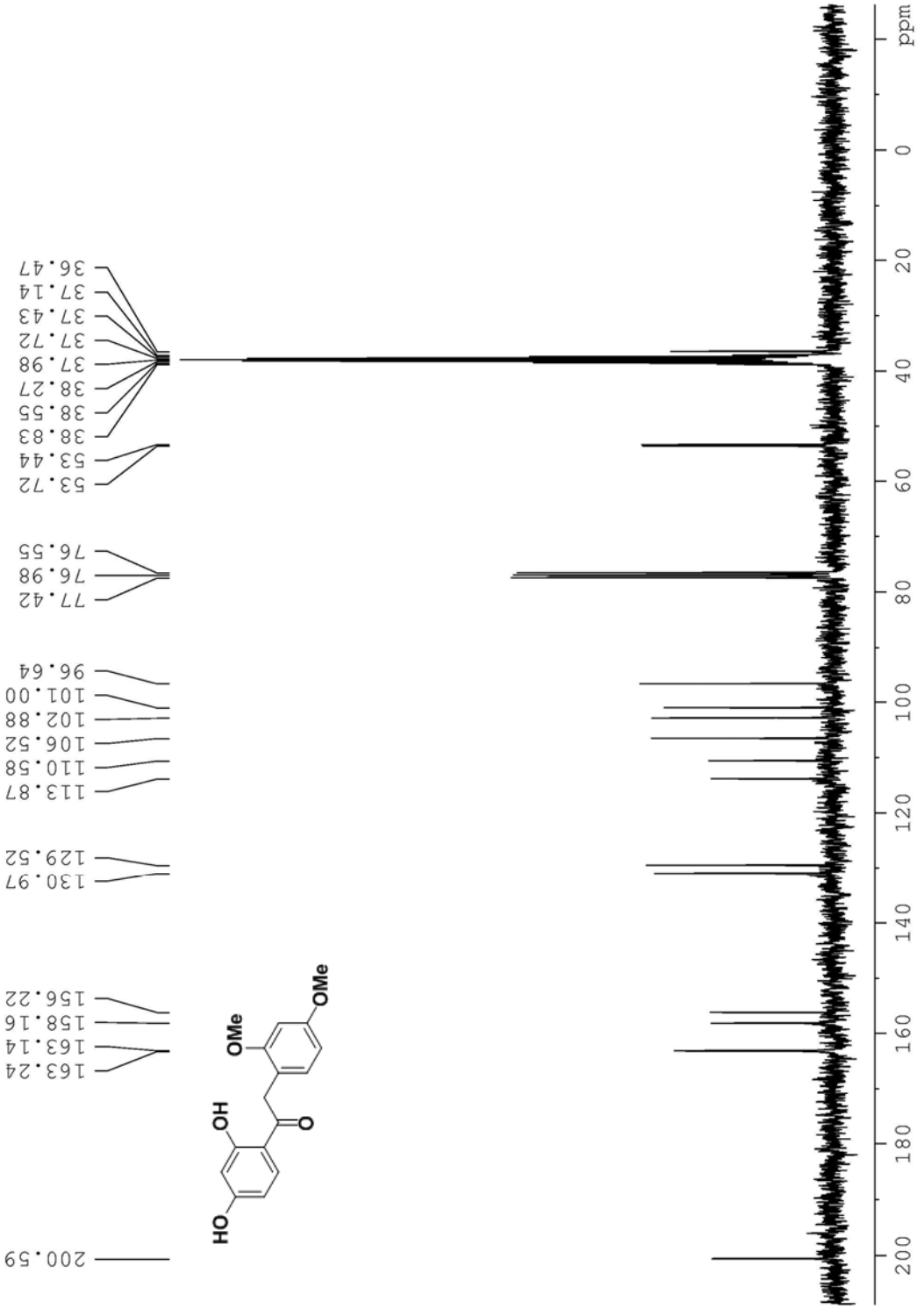

Figure S16. ^{13}C NMR spectrum of **3a** in $CDCl_3$ + DMSO-d_6

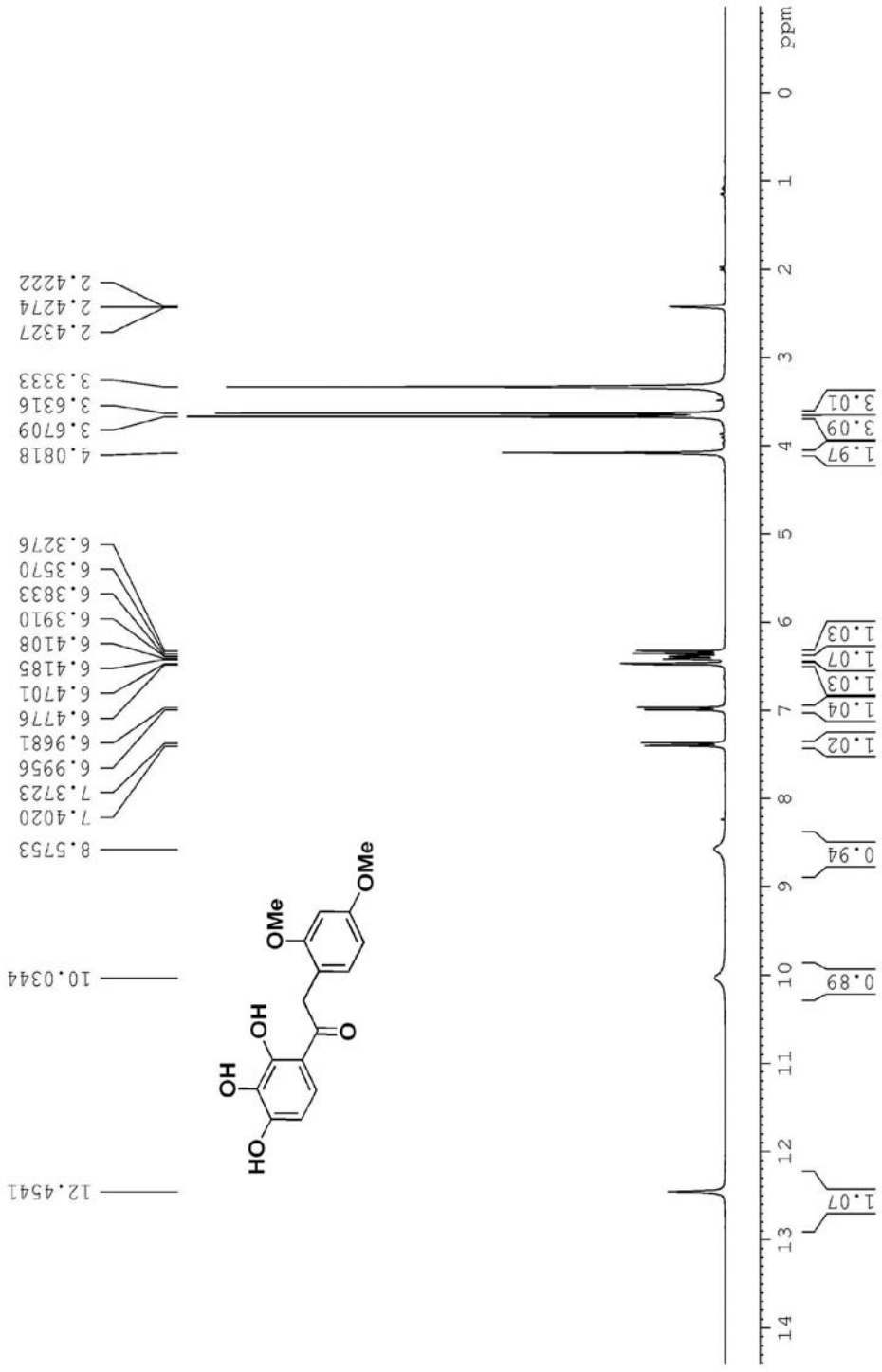

Figure S17. ^{1}H NMR spectrum of **3b** in DMSO-d_6.

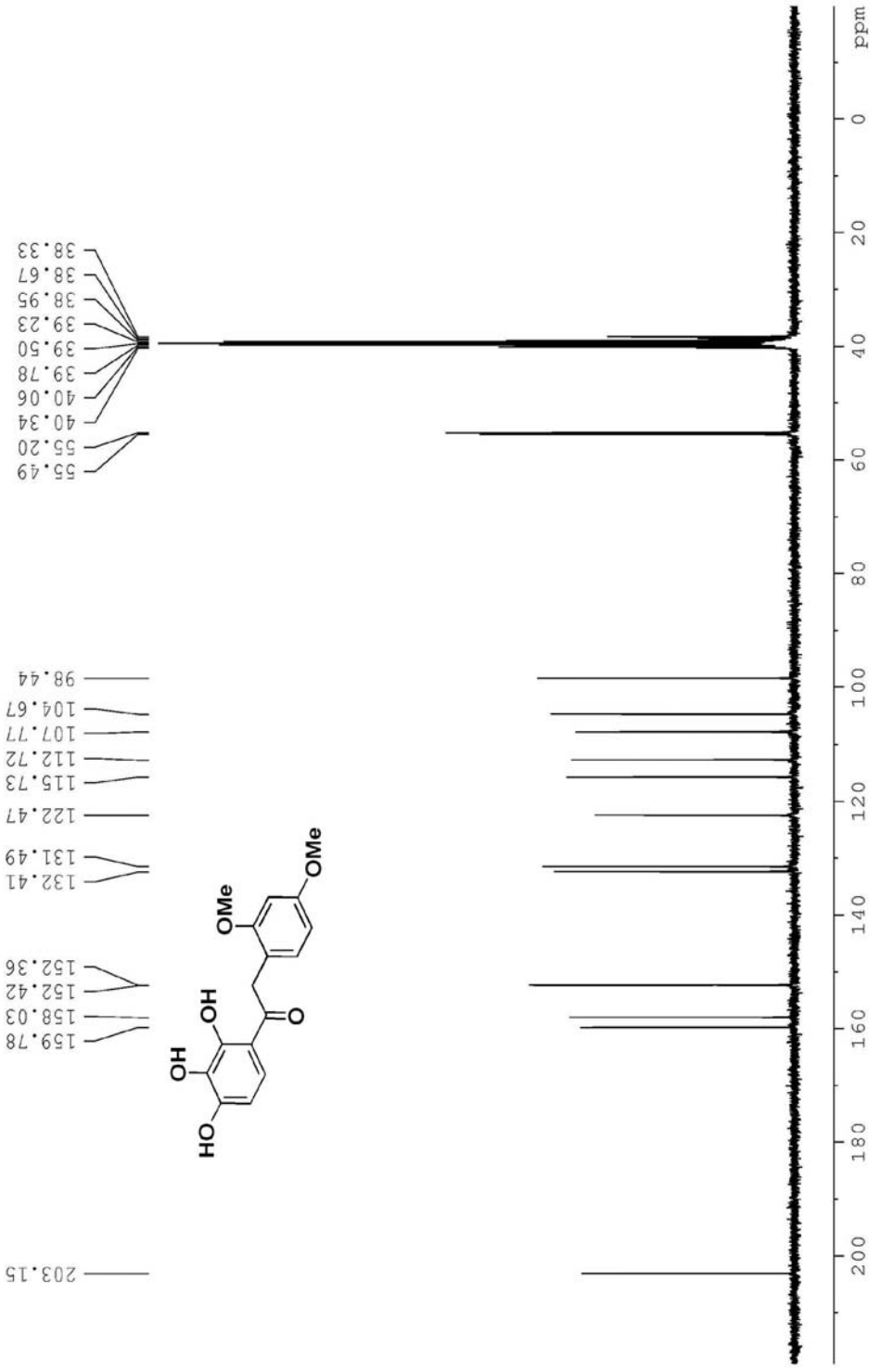

Figure S18. ^{13}C NMR spectrum of **3b** in DMSO-d_6

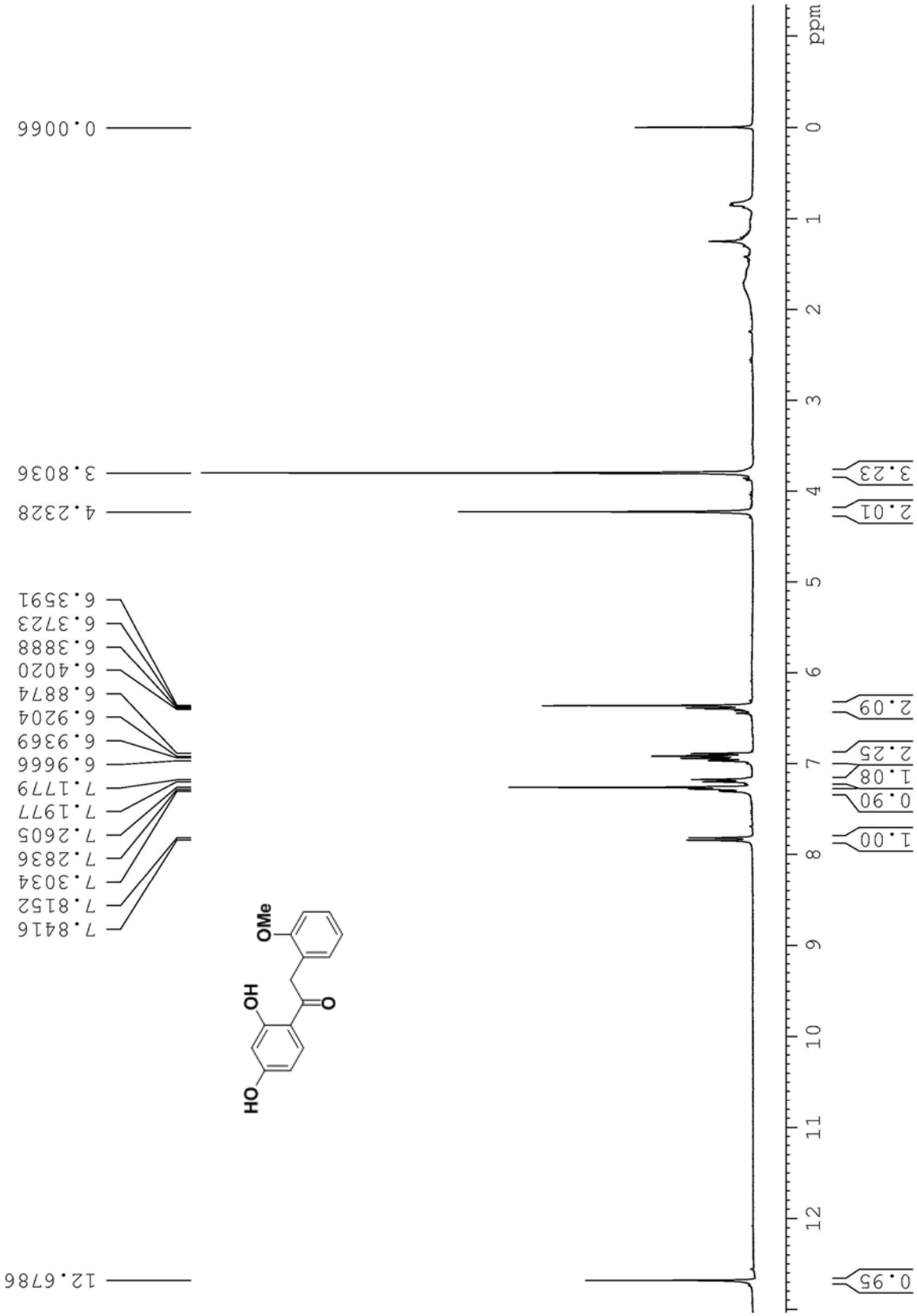

Figure S19. ^{1}H NMR spectrum of **3c** in $CDCl_3$

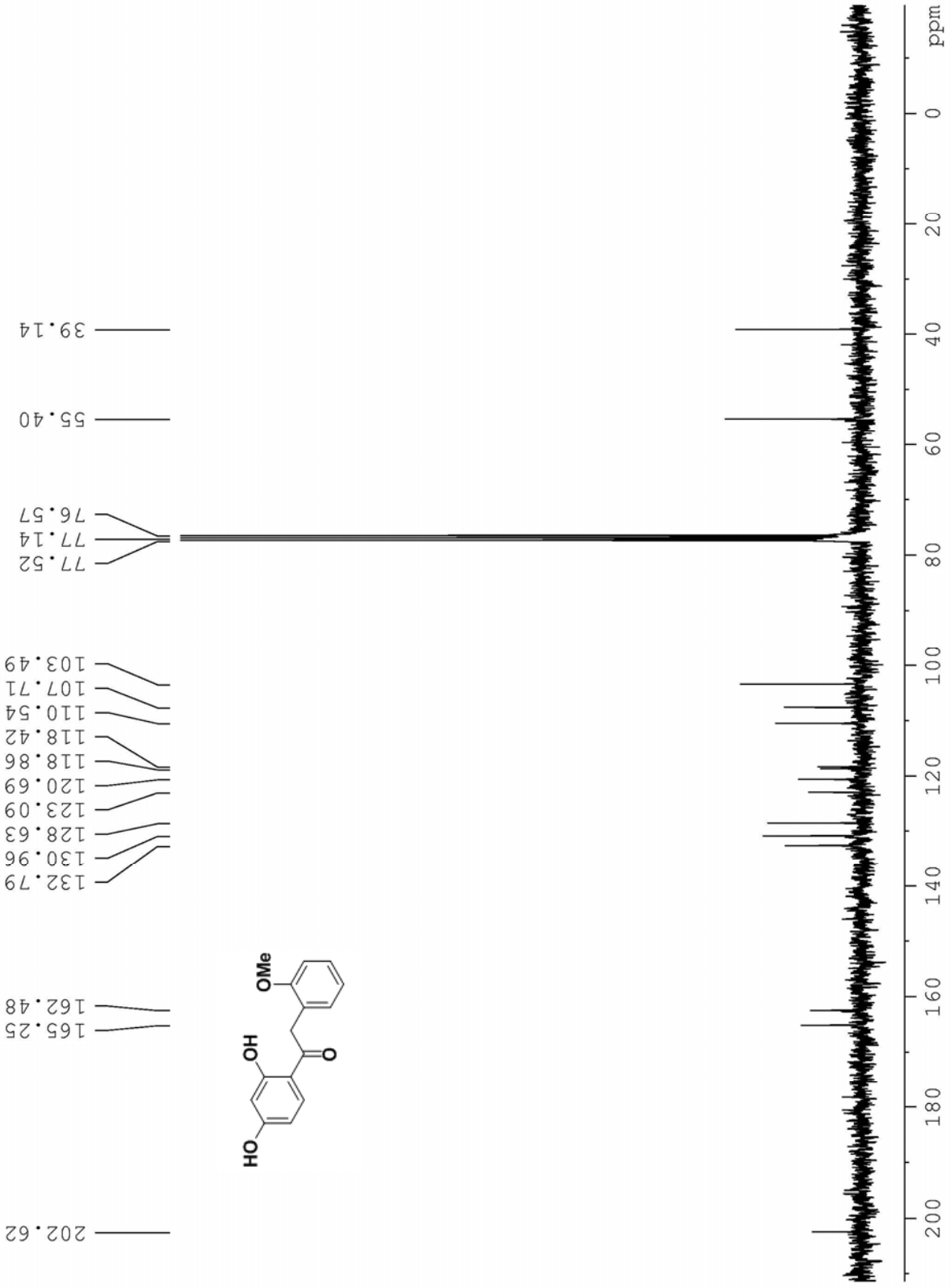

Figure S20. ^{13}C NMR spectrum of **3c** in $CDCl_3$

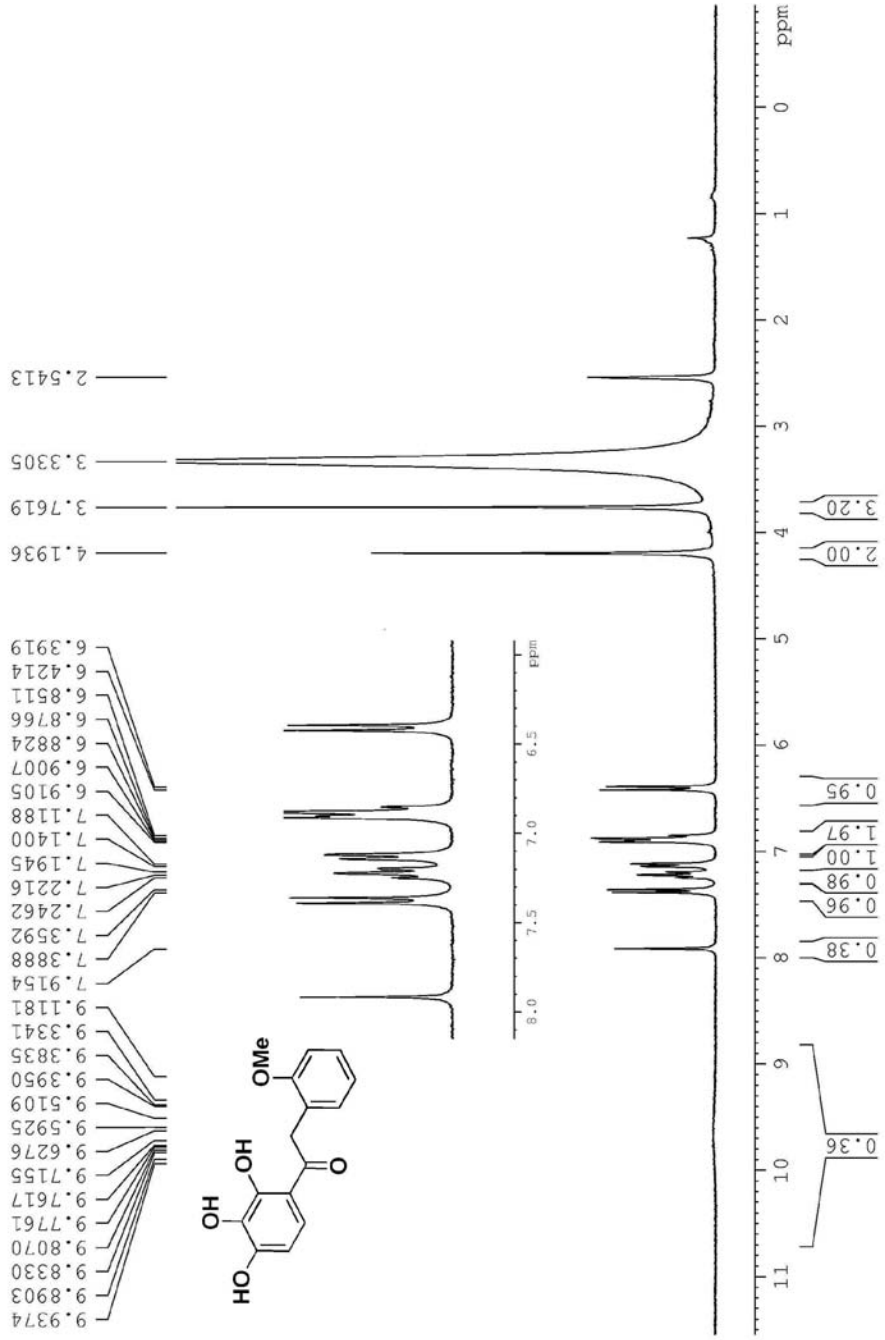

Figure S21. ^{1}H NMR spectrum of **3d** in $CDCl_3$ + DMSO-d_6

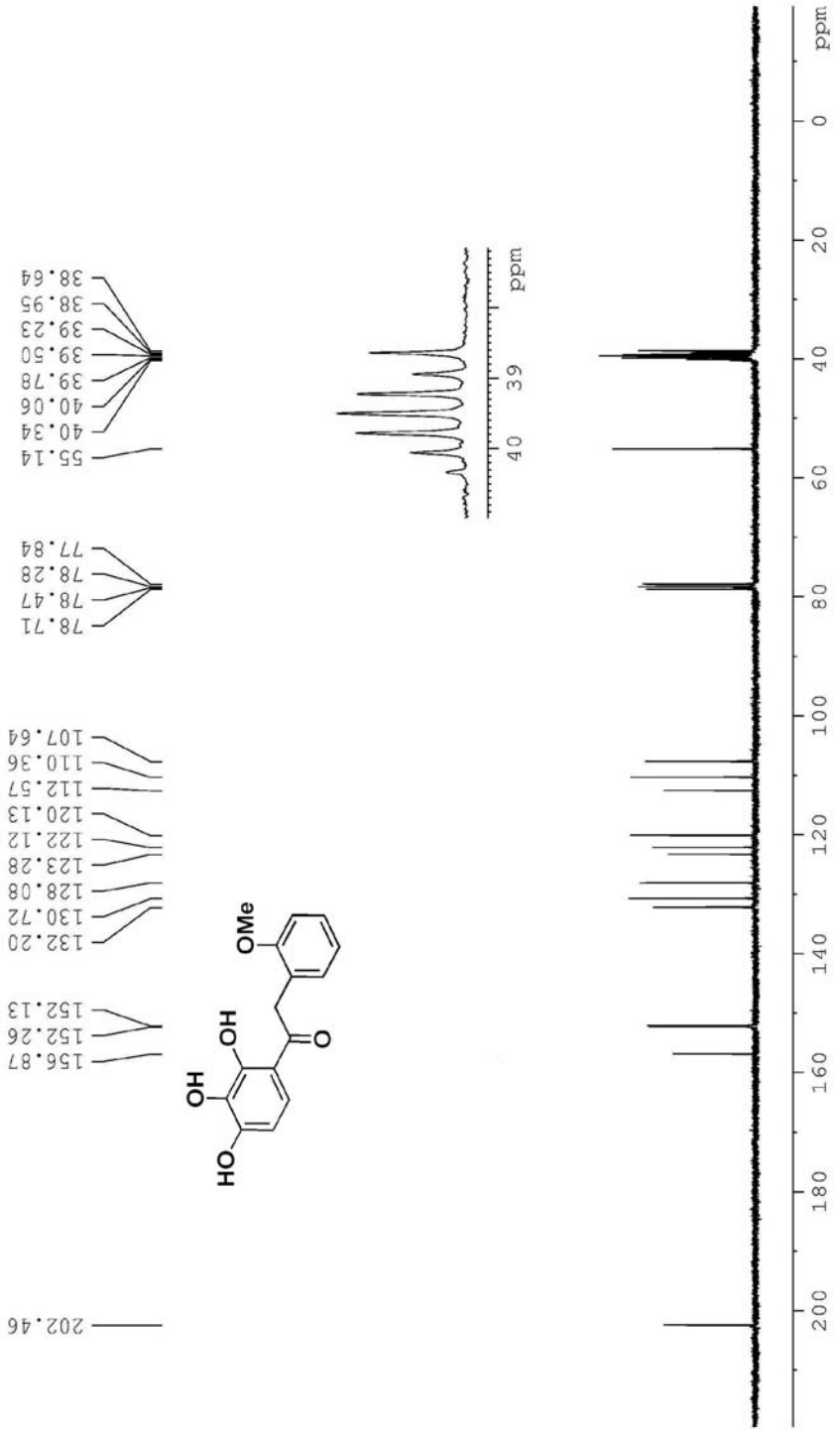

Figure S22. ^{13}C NMR spectrum of **3d** in $CDCl_3$ + DMSO-d_6

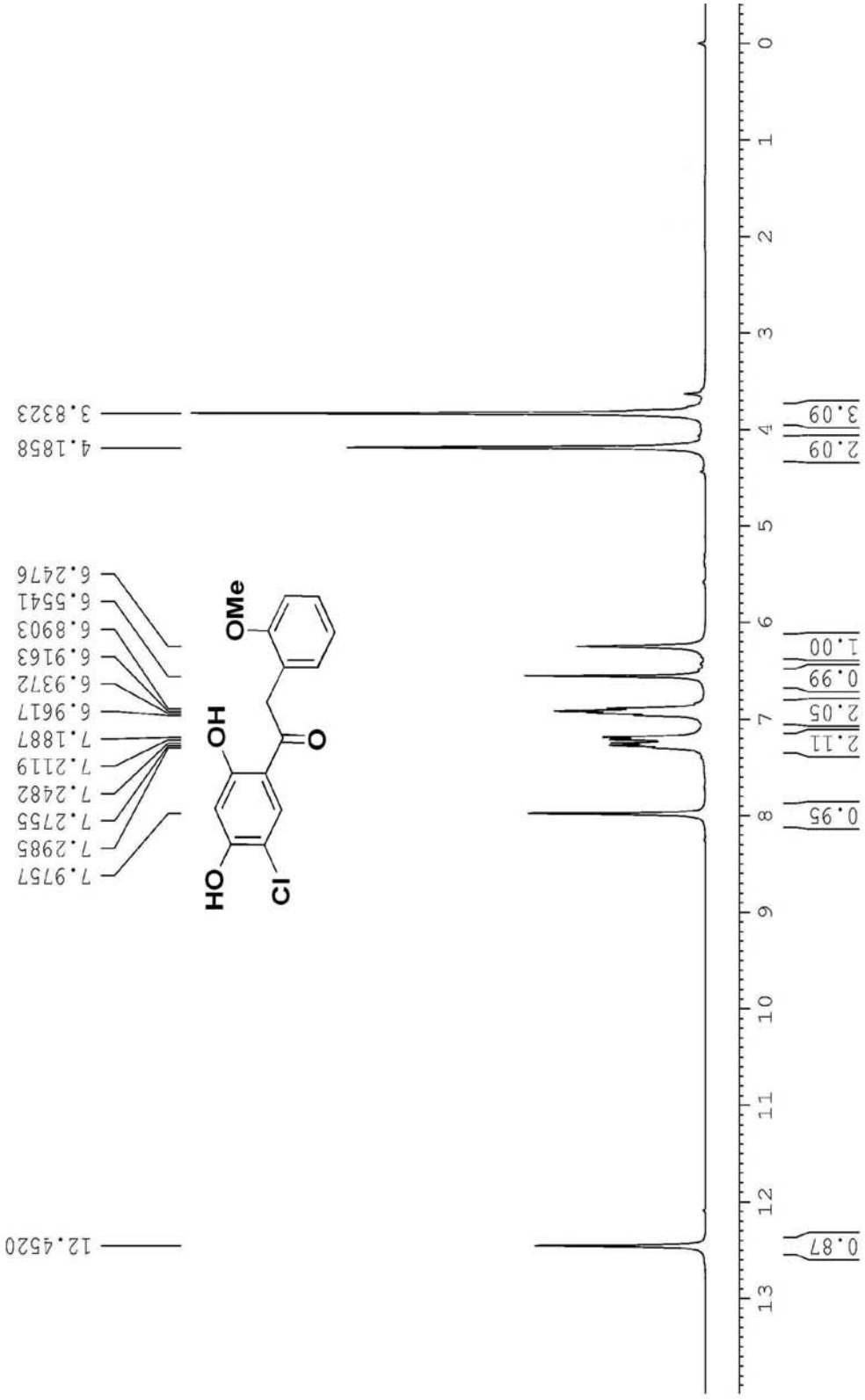

Figure S23. ^{1}H NMR spectrum of **3e** in $CDCl_3$

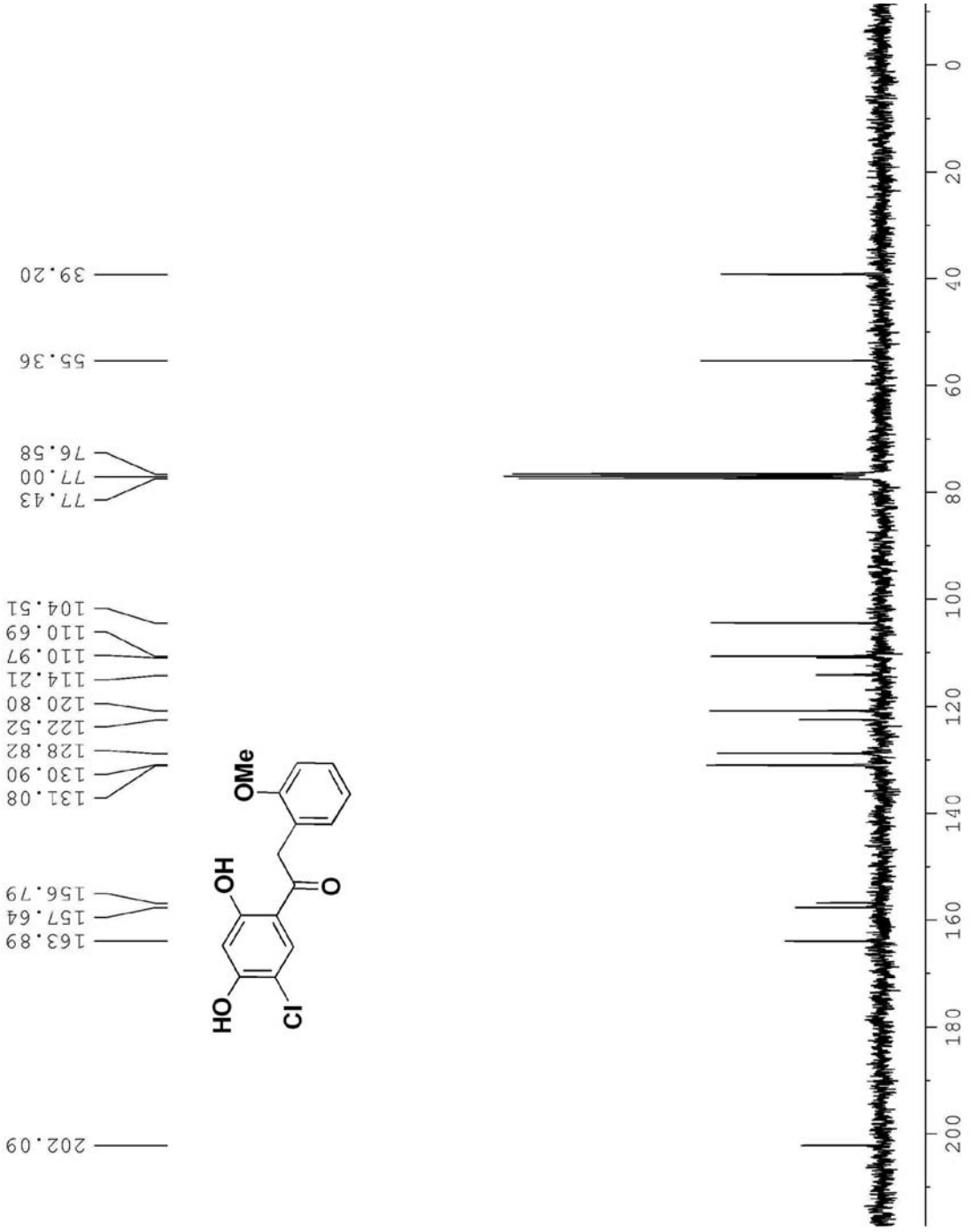

Figure S24. ^{13}C NMR spectrum of **3e** in $CDCl_3$

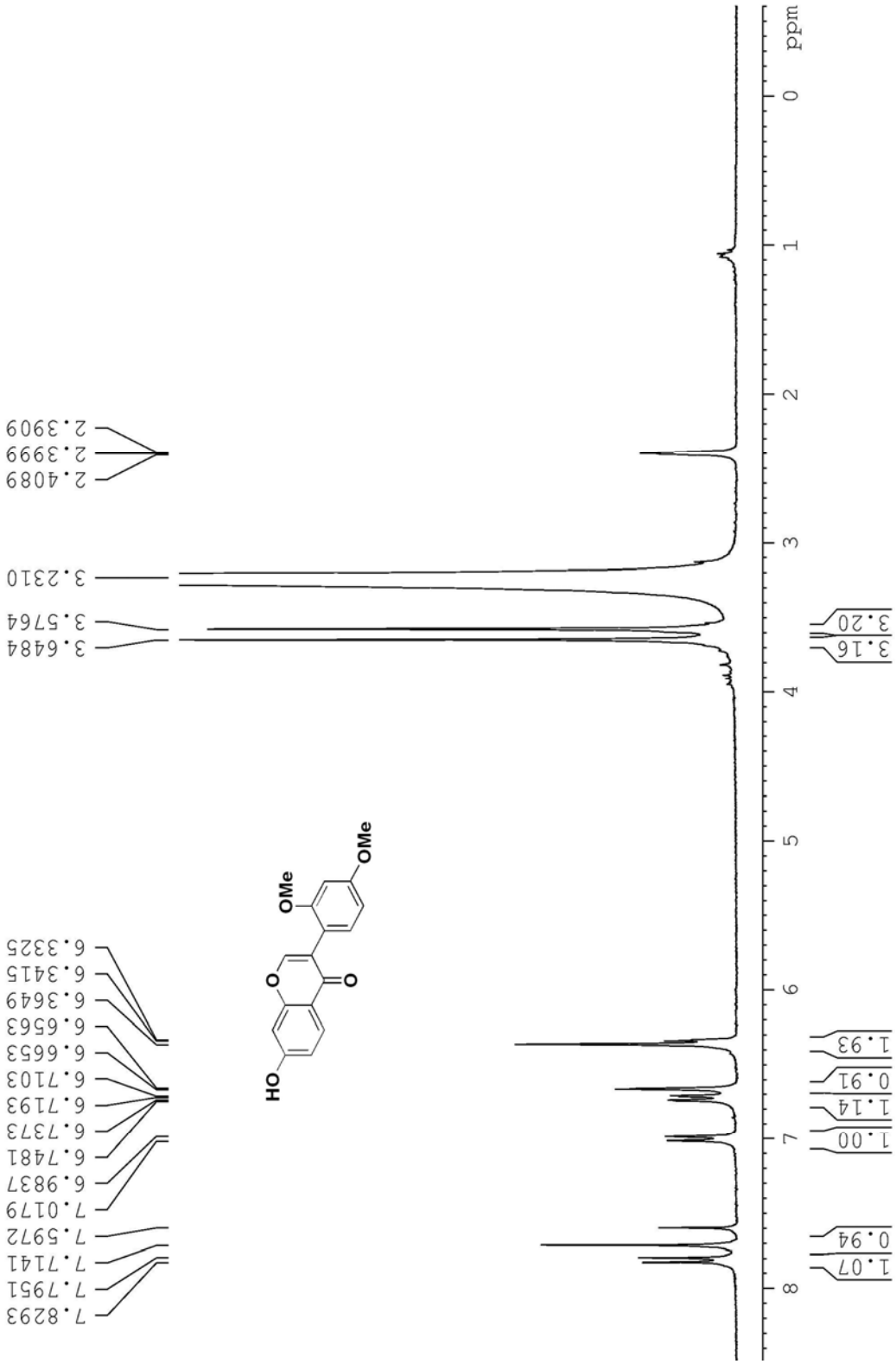

Figure S25. ^{1}H NMR spectrum of **4a** in $CDCl_3$ + DMSO-d_6

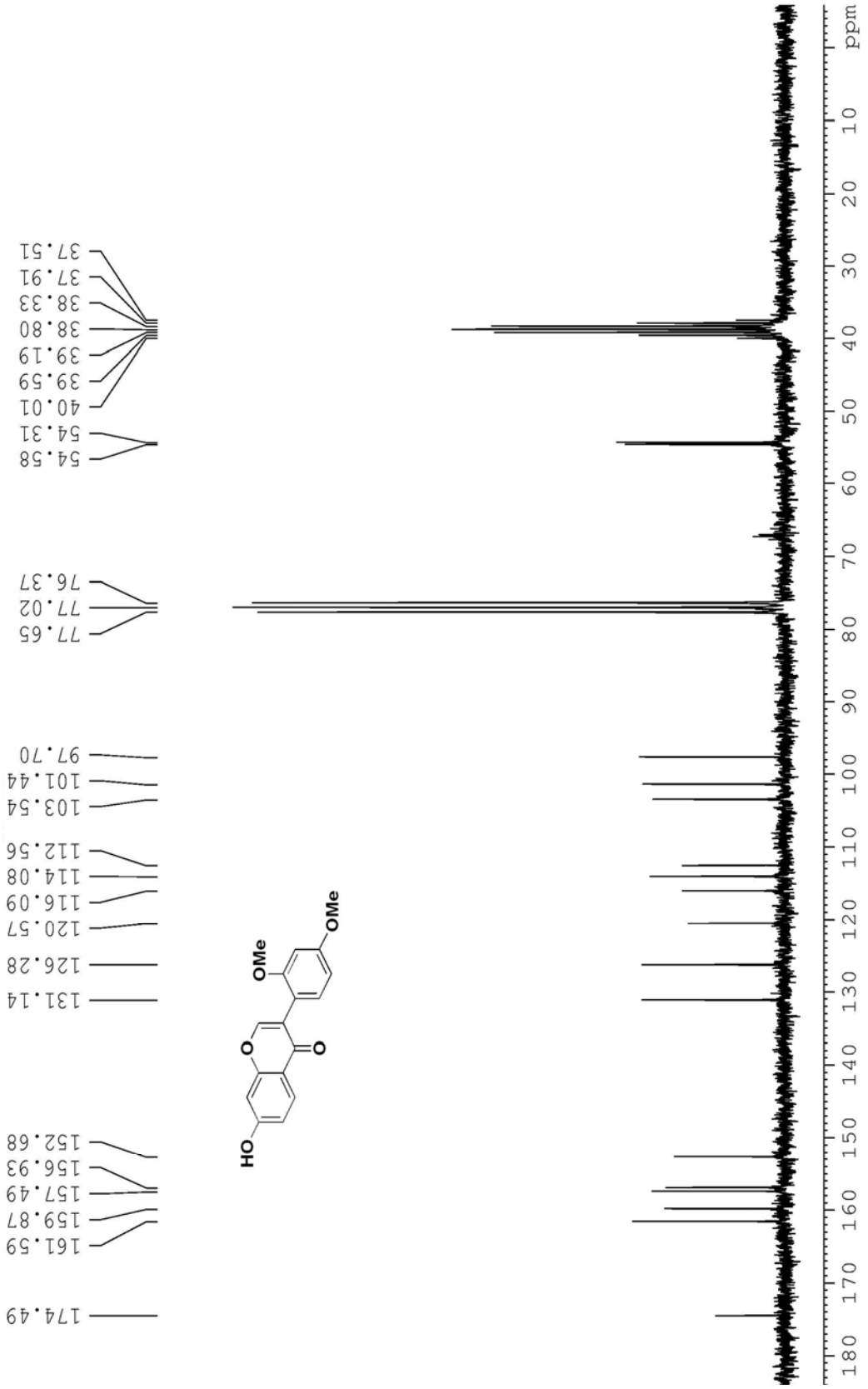

Figure S26. ^{13}C NMR spectrum of **4a** in $CDCl_3$ + DMSO-d_6

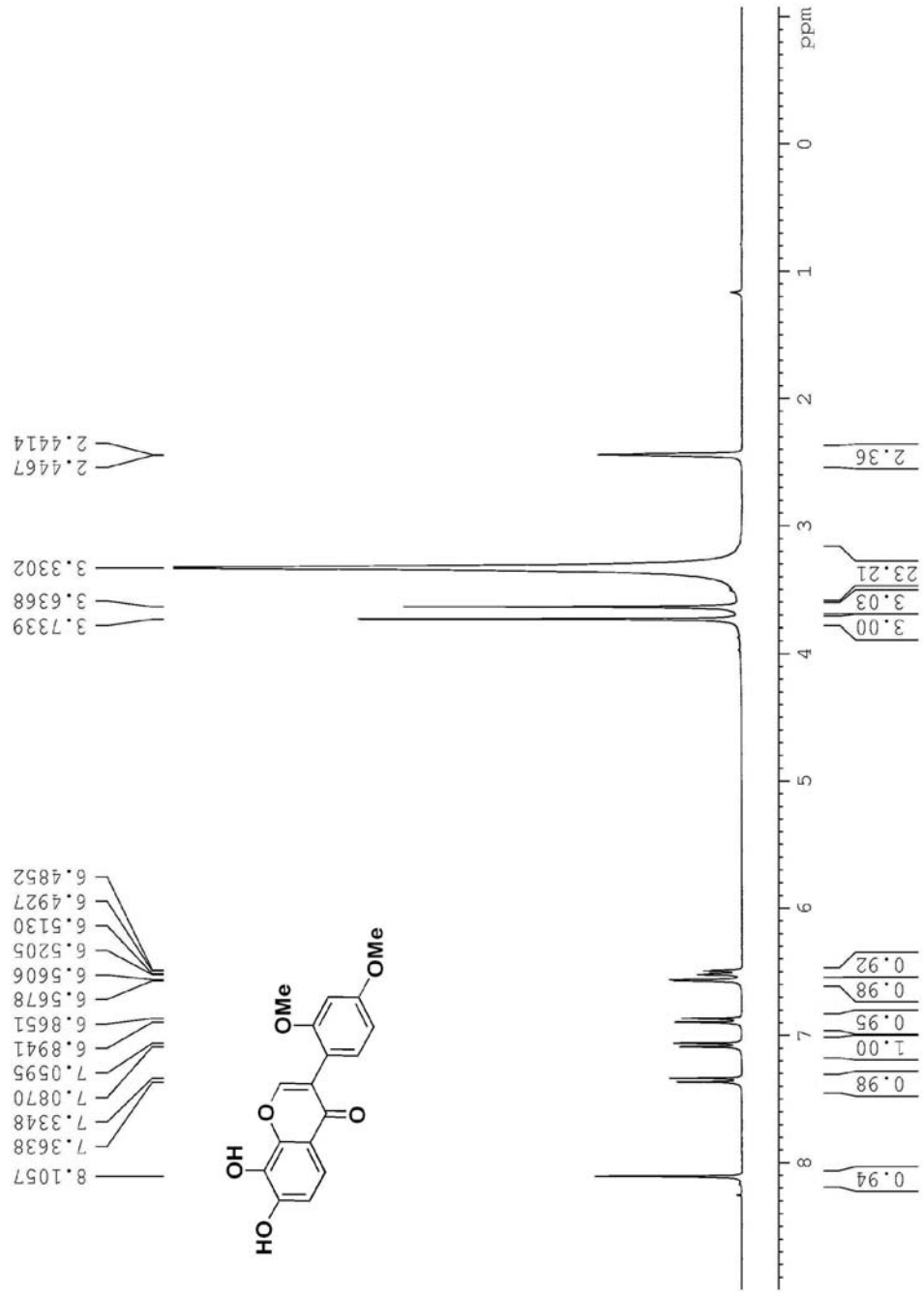

Figure S27. ^{1}H NMR spectrum of **4b** in DMSO-d_6

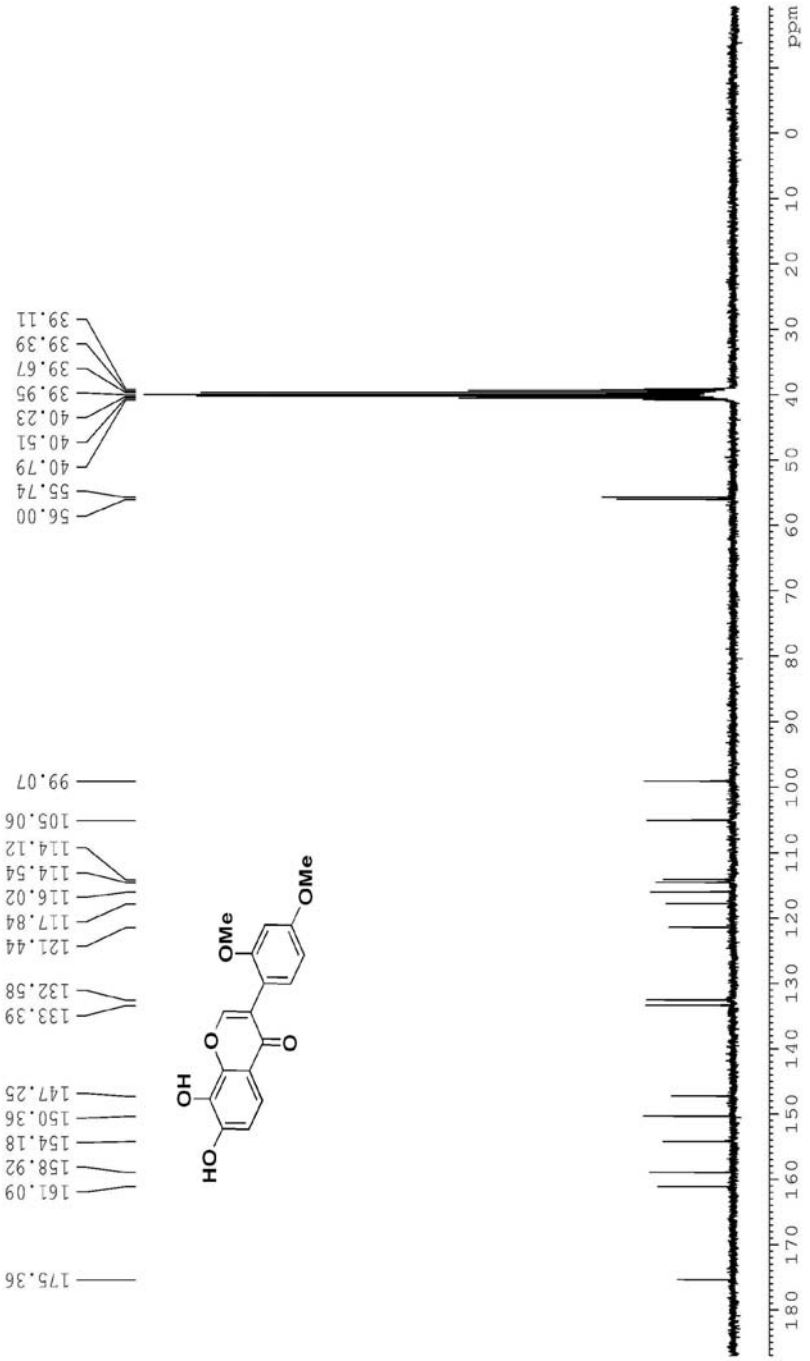

Figure S28. ^{13}C NMR spectrum of **4b** in DMSO-d_6

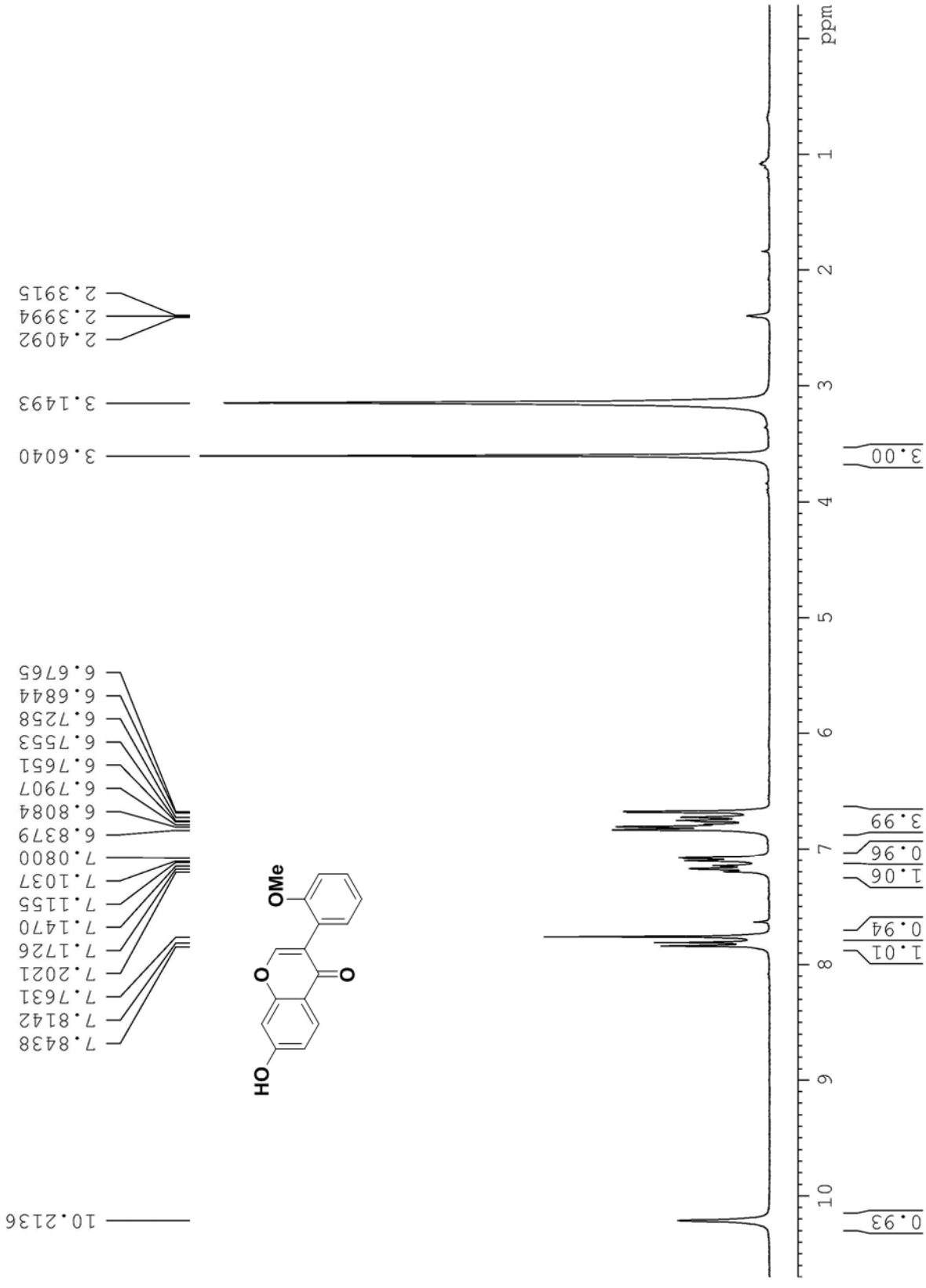

Figure S29. ^{1}H NMR spectrum of **4c** in $CDCl_3$ + DMSO-d_6

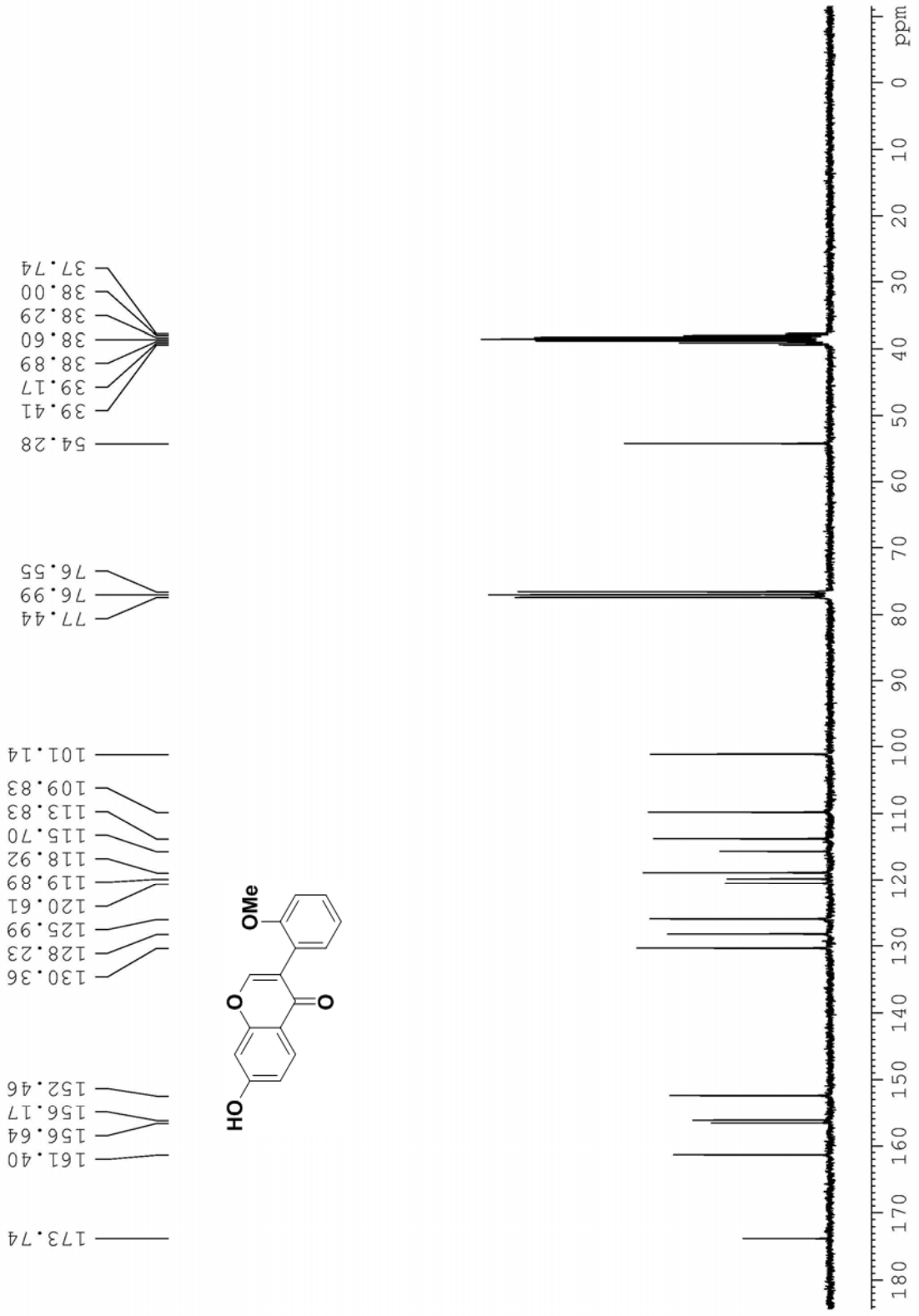

Figure S30. ^{13}C NMR spectrum of **4c** in $CDCl_3$ + DMSO-d_6

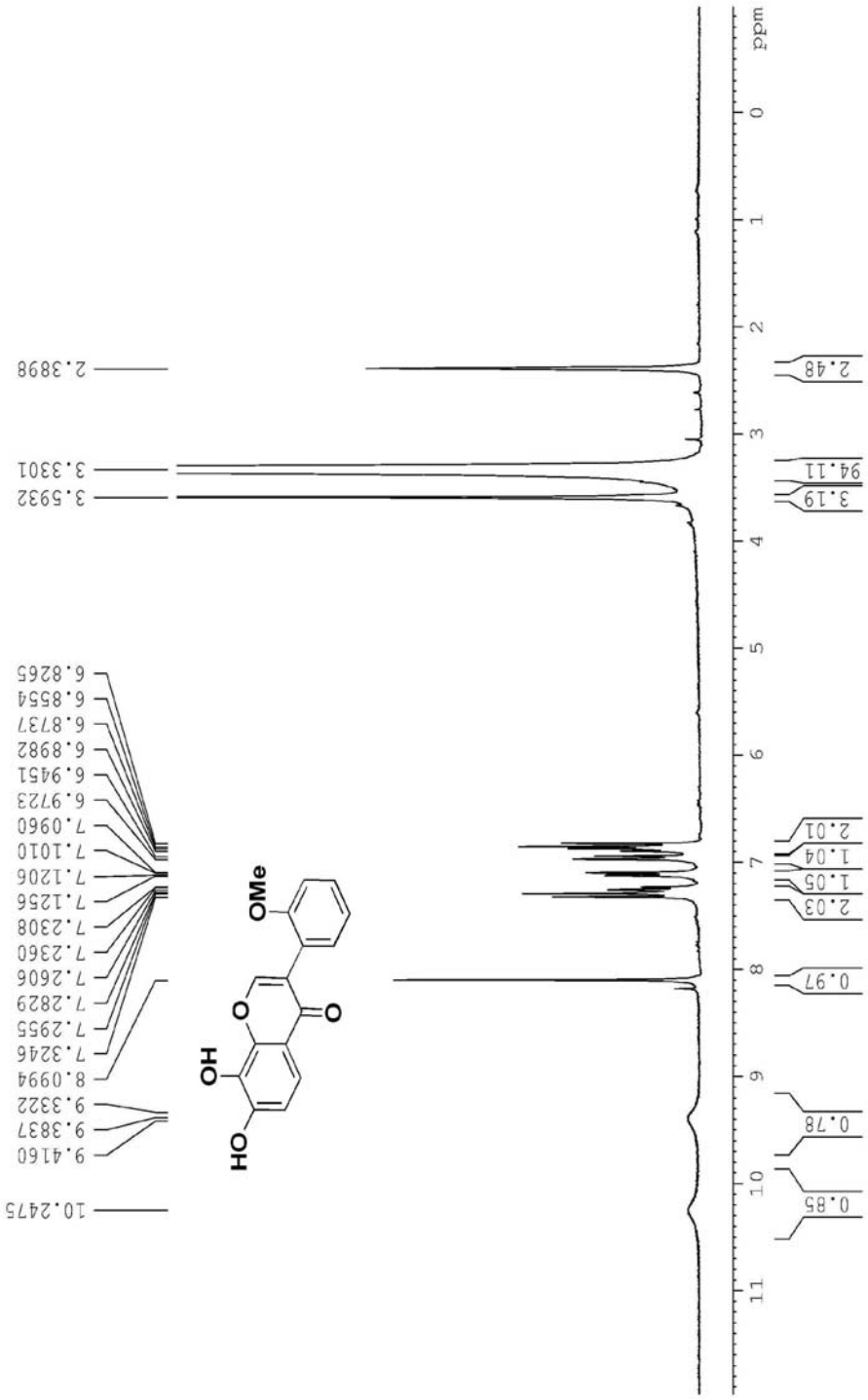

Figure S31. ^{1}H NMR spectrum of **4d** in DMSO-d_6

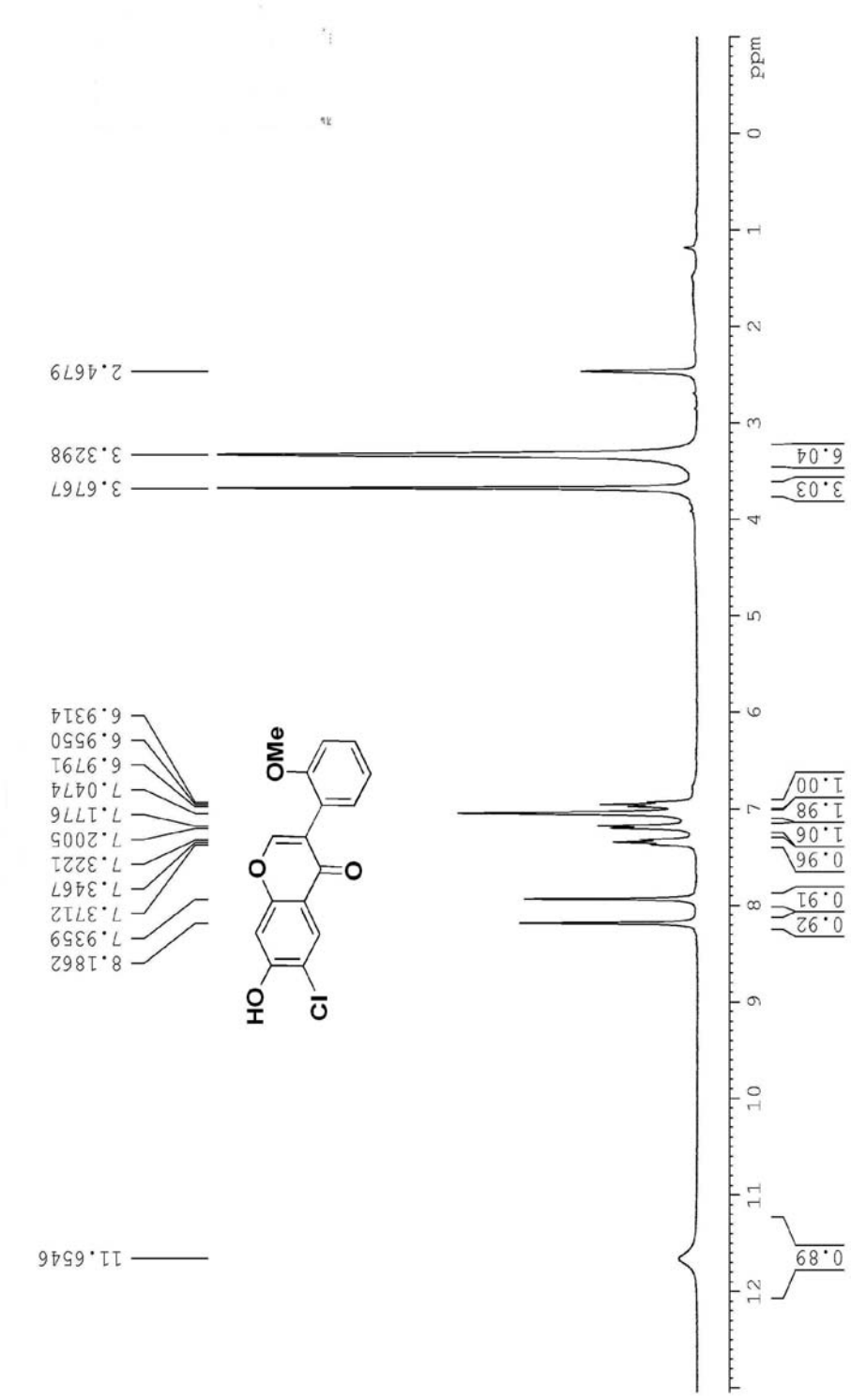

Figure S32. ^{1}H NMR spectrum of **4e** in DMSO-d_6

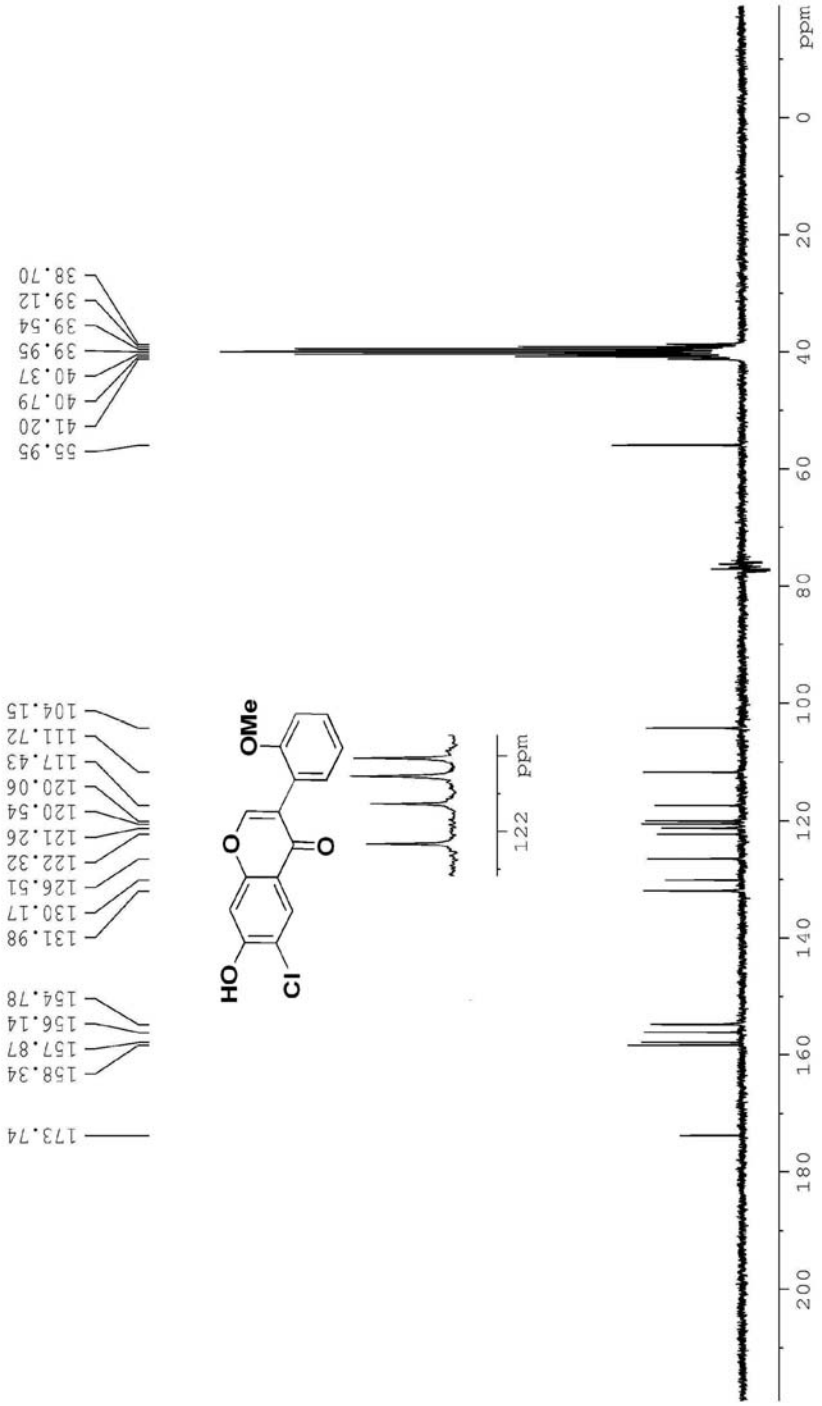

Figure S33. ^{13}C NMR spectrum of **4e** in DMSO-d_6

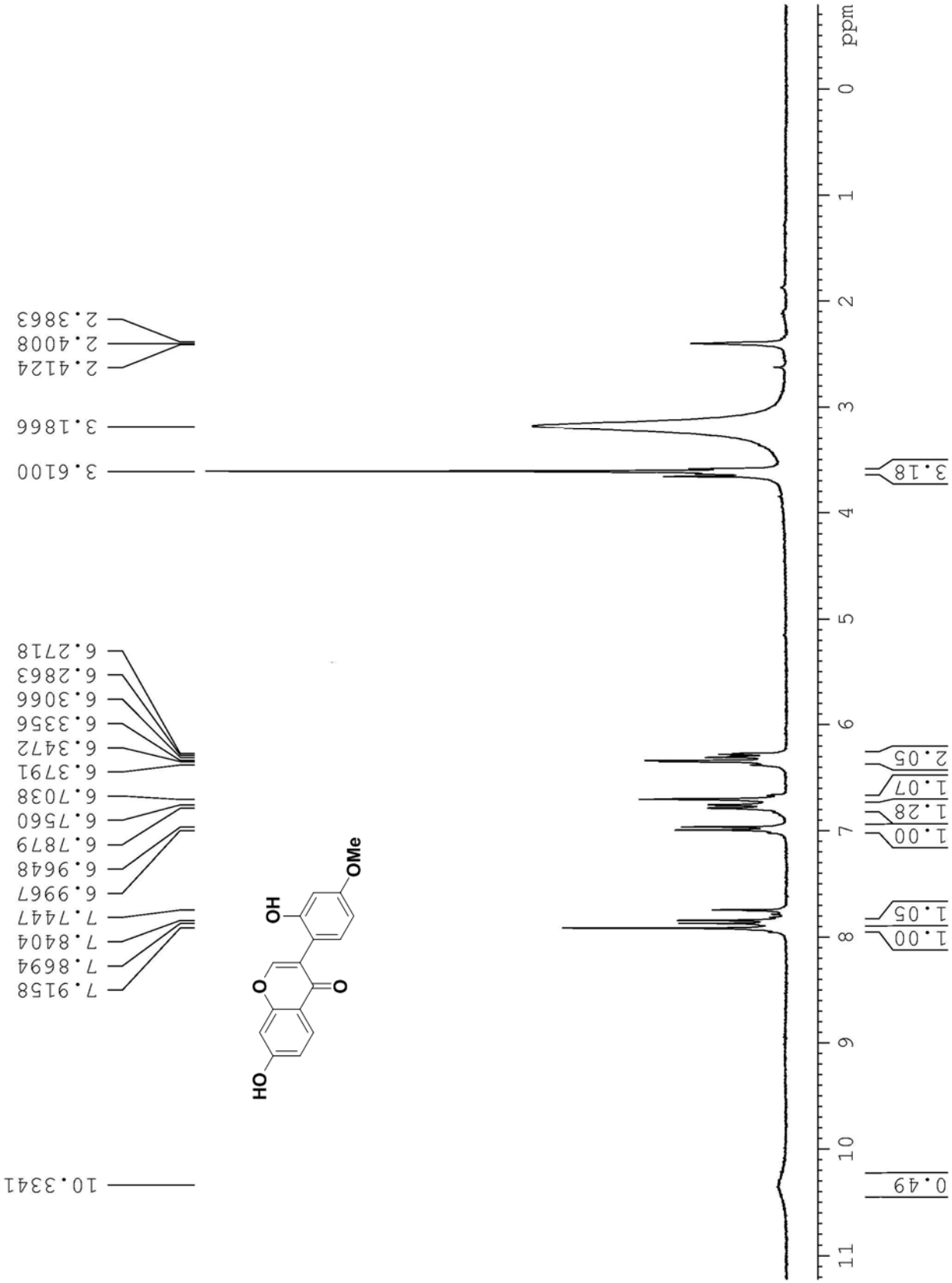

Figure S34. ^{1}H NMR spectrum of **5a** in $CDCl_3$ + DMSO-d_6

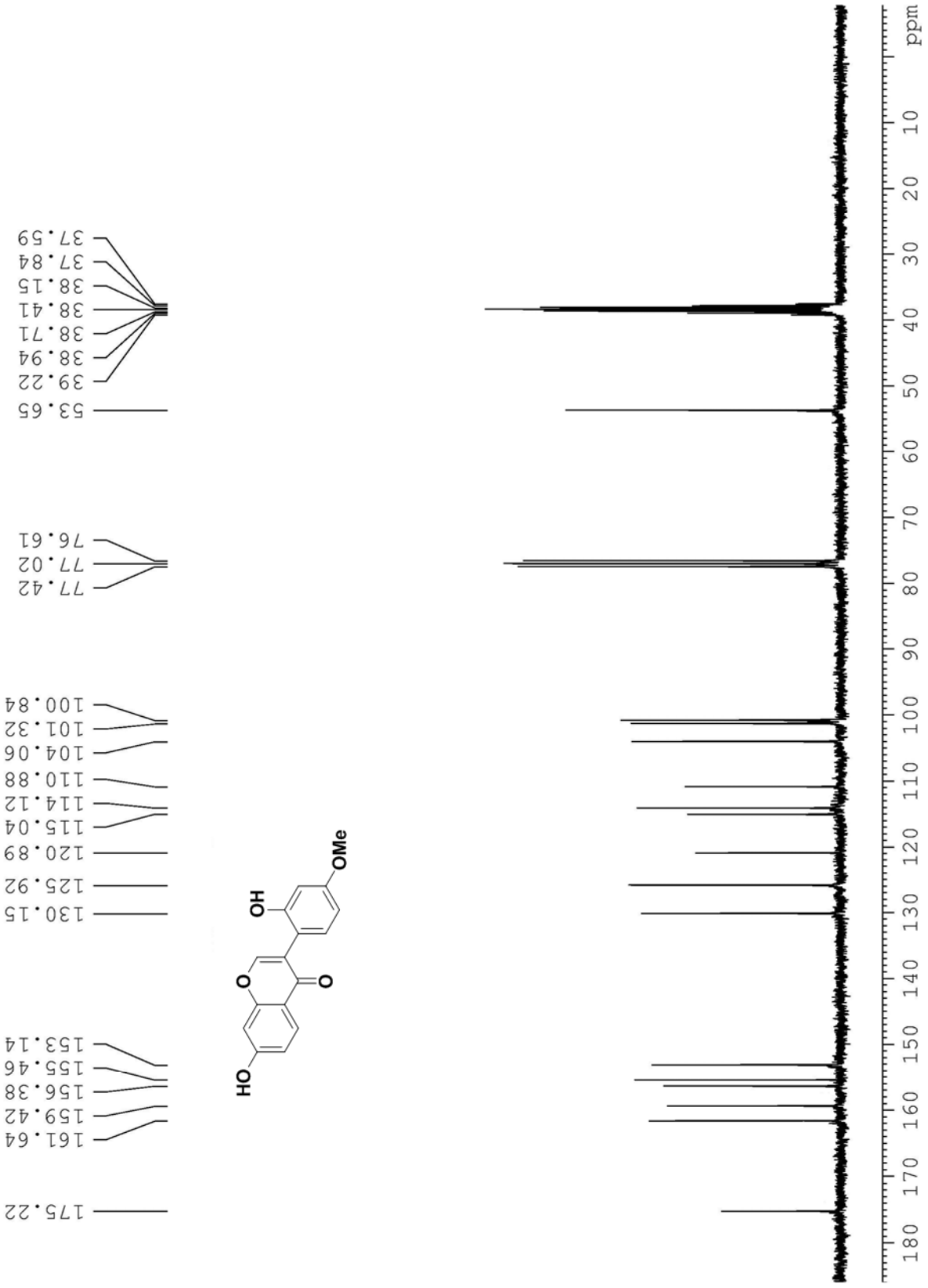

Figure S35. ^{13}C NMR spectrum of 5a in $CDCl_3$ + DMSO-d_6

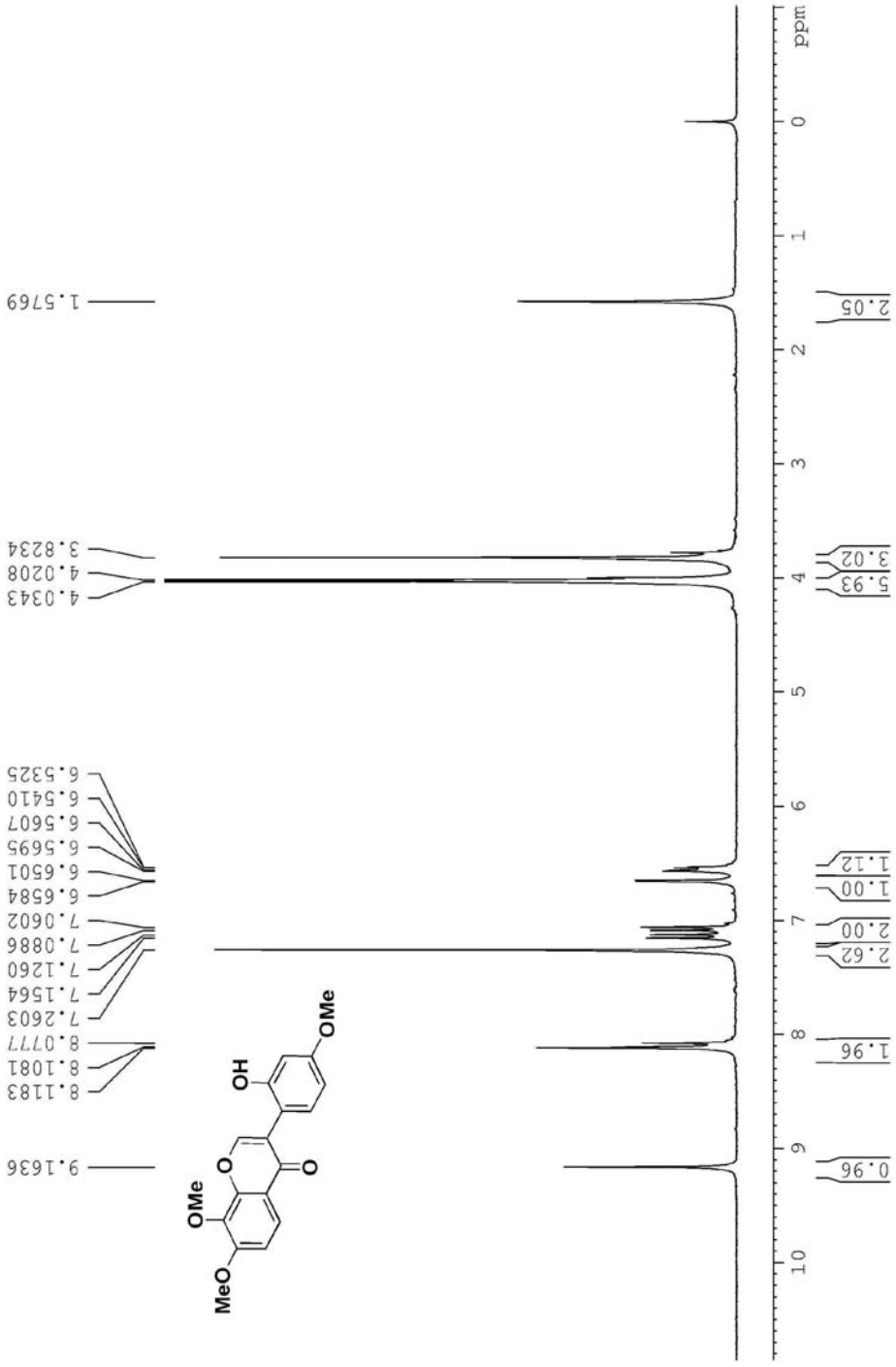

Figure S36. ^{1}H NMR spectrum of **5b** in $CDCl_3$

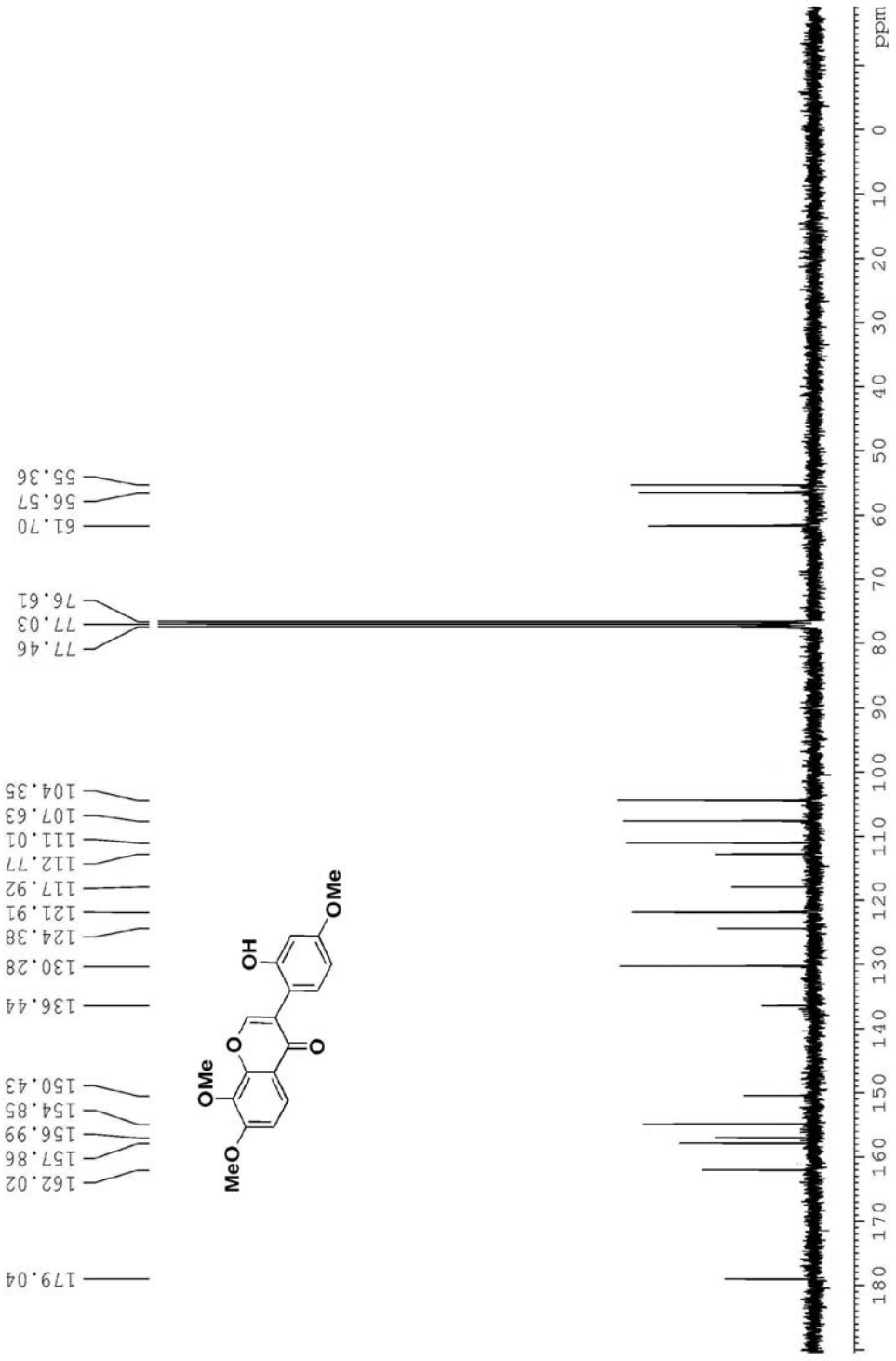

Figure S37. ^{13}C NMR spectrum of **5b** in $CDCl_3$

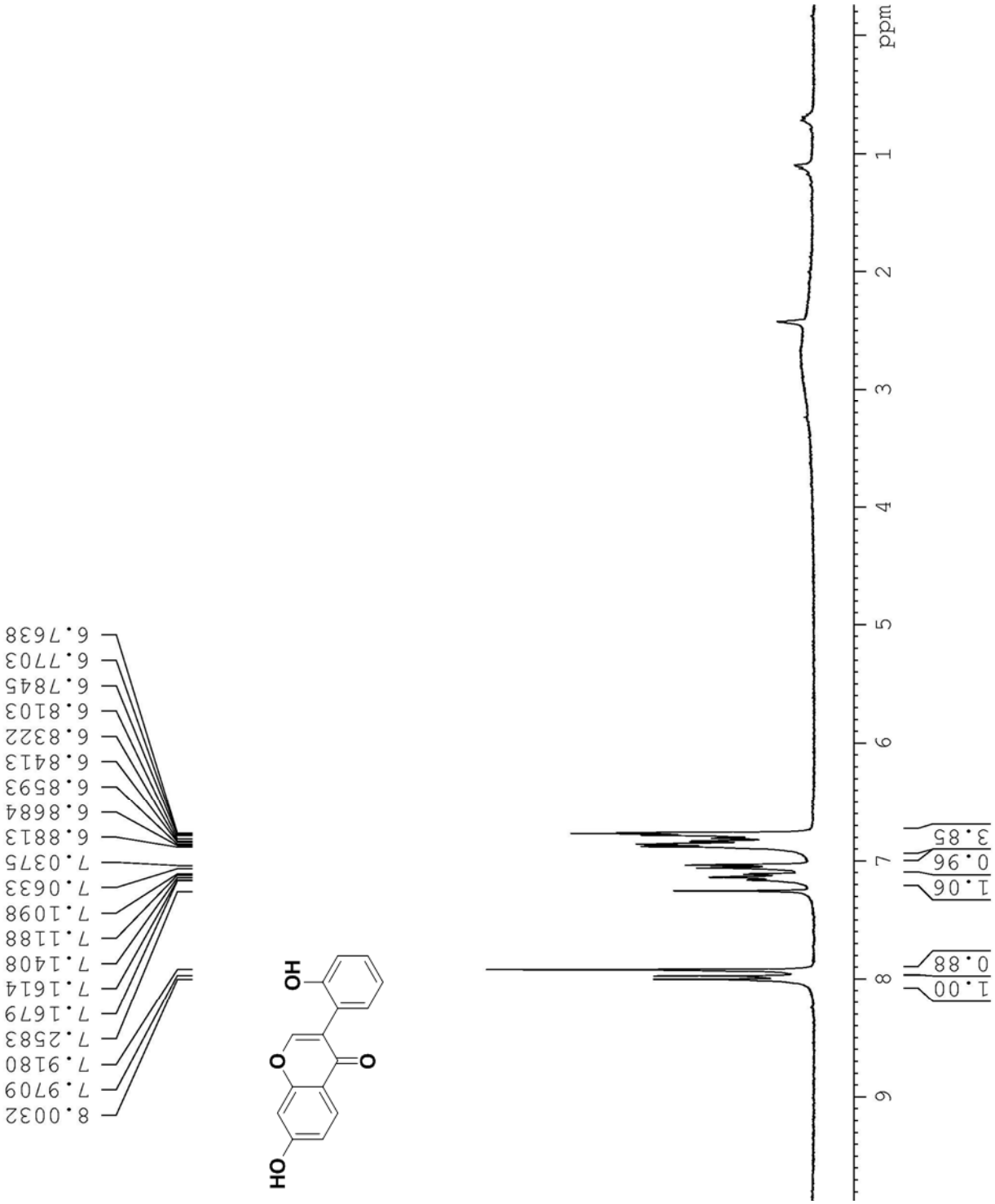

Figure S38. ^{1}H NMR spectrum of **5c** in $CDCl_3$

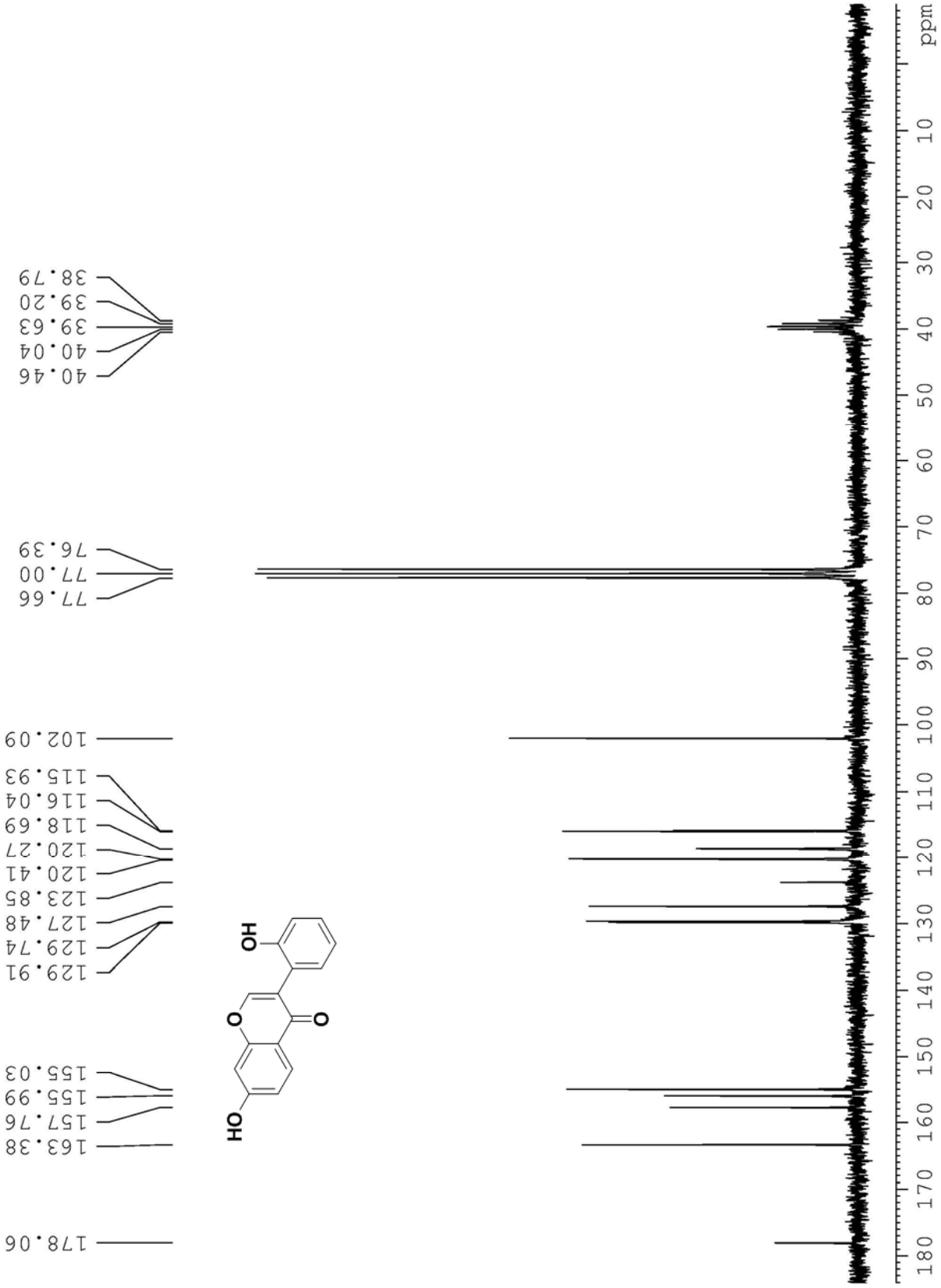

Figure S39. ^{13}C NMR spectrum of **5c** in $CDCl_3$ + DMSO-d_6

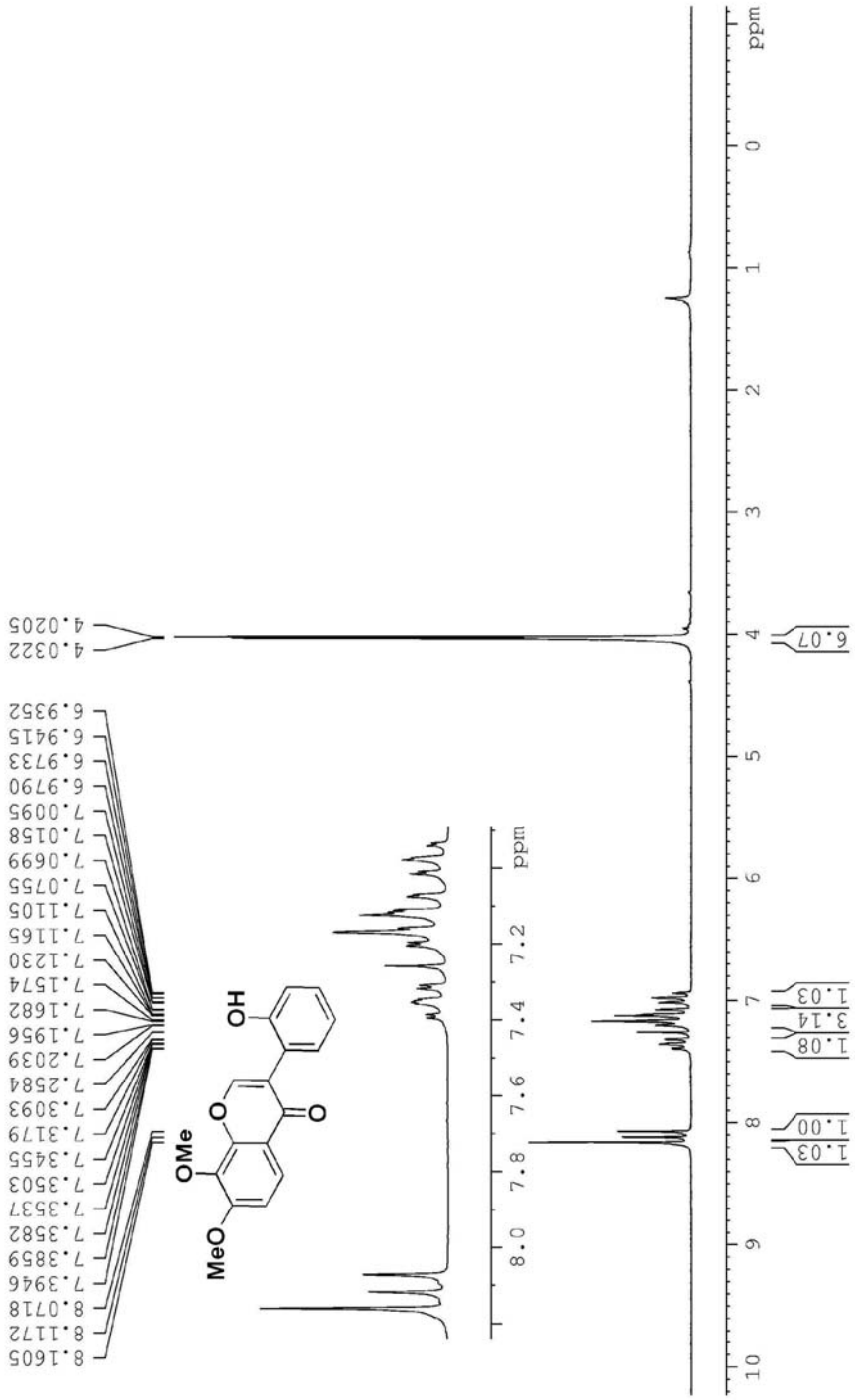

Figure S40. ^{1}H NMR spectrum of **5d** in $CDCl_3$

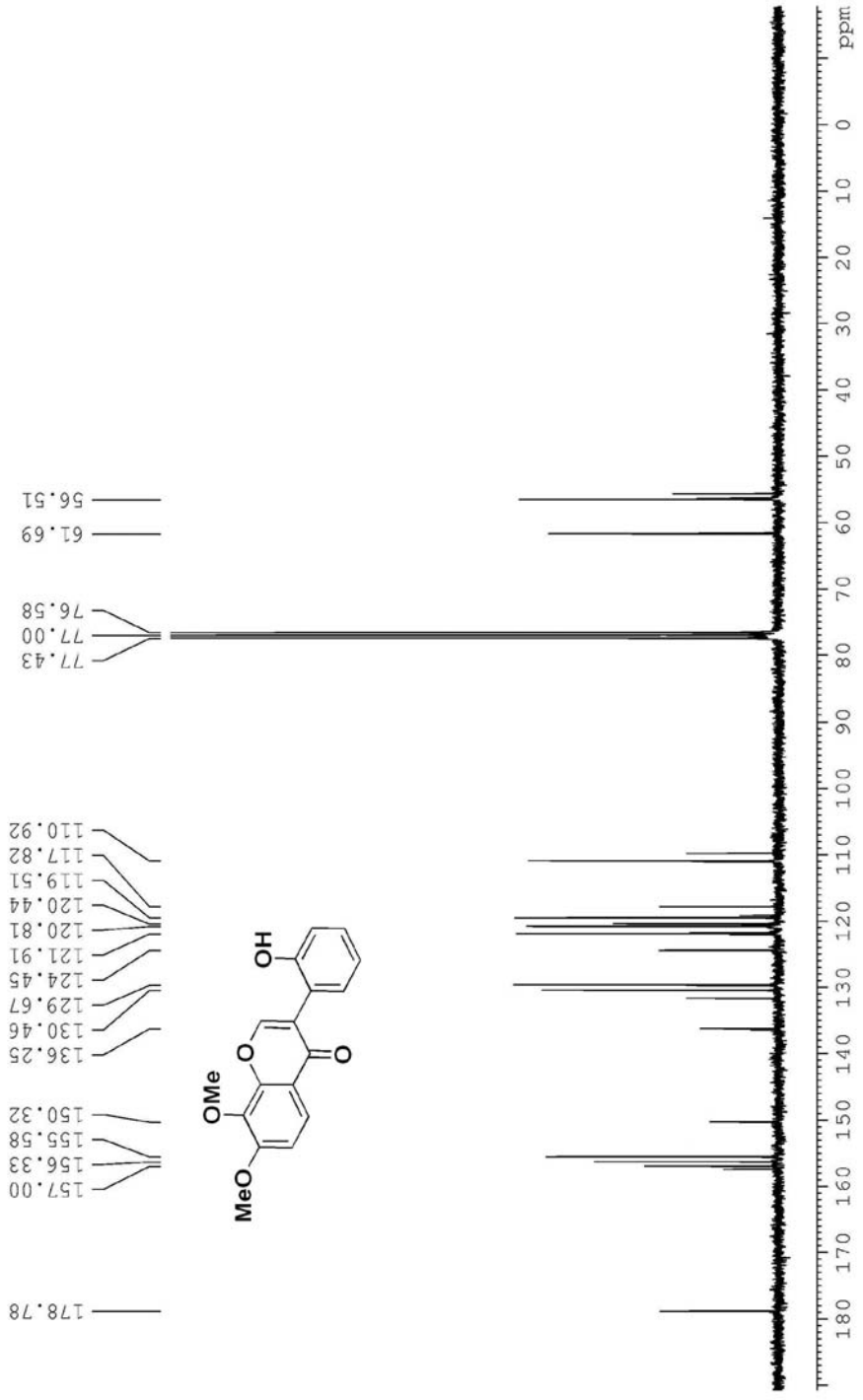

Figure S41. ^{13}C NMR spectrum of **5d** in $CDCl_3$

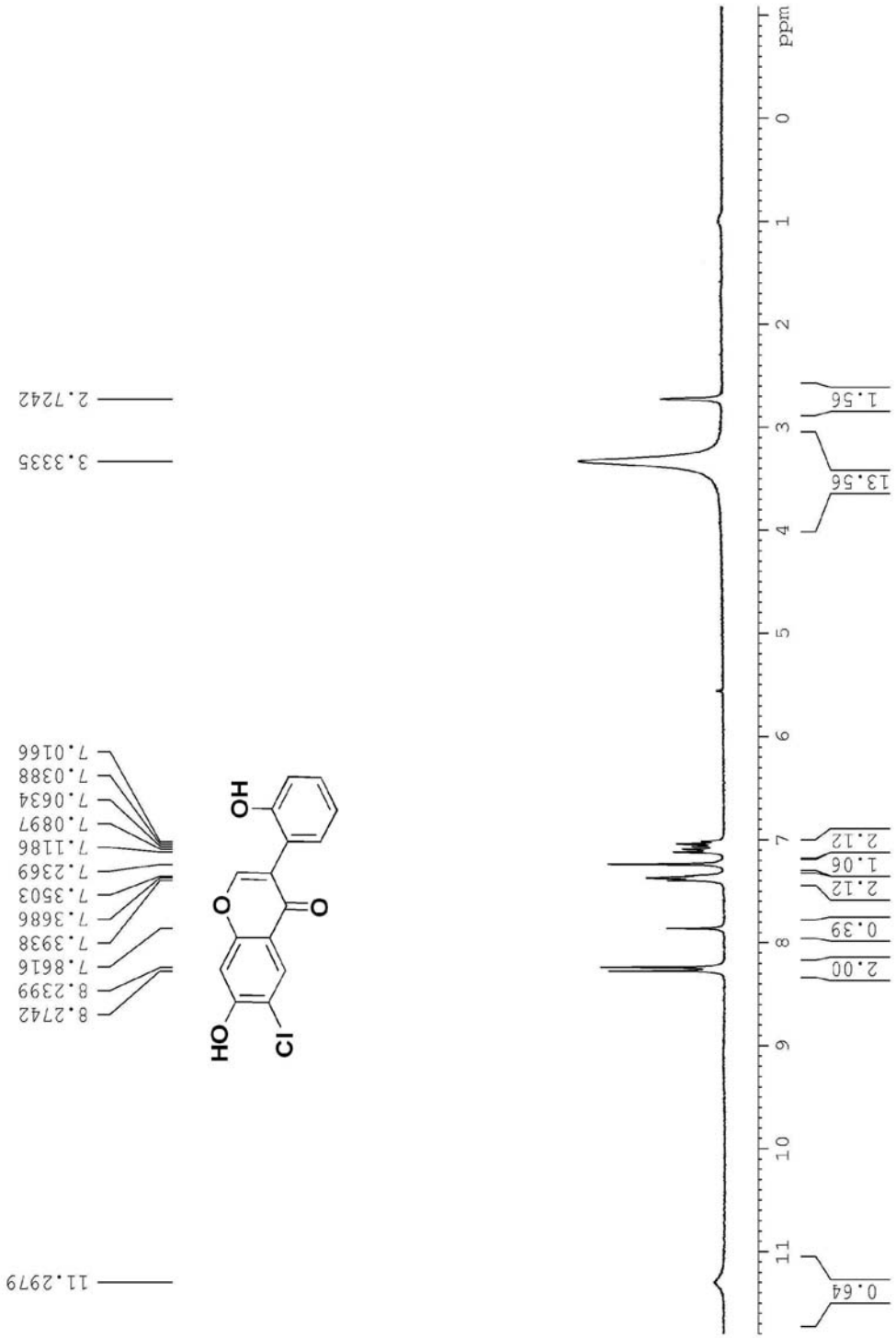

Figure S42. ^{1}H NMR spectrum of **5e** in $CDCl_3$ + DMSO-d_6

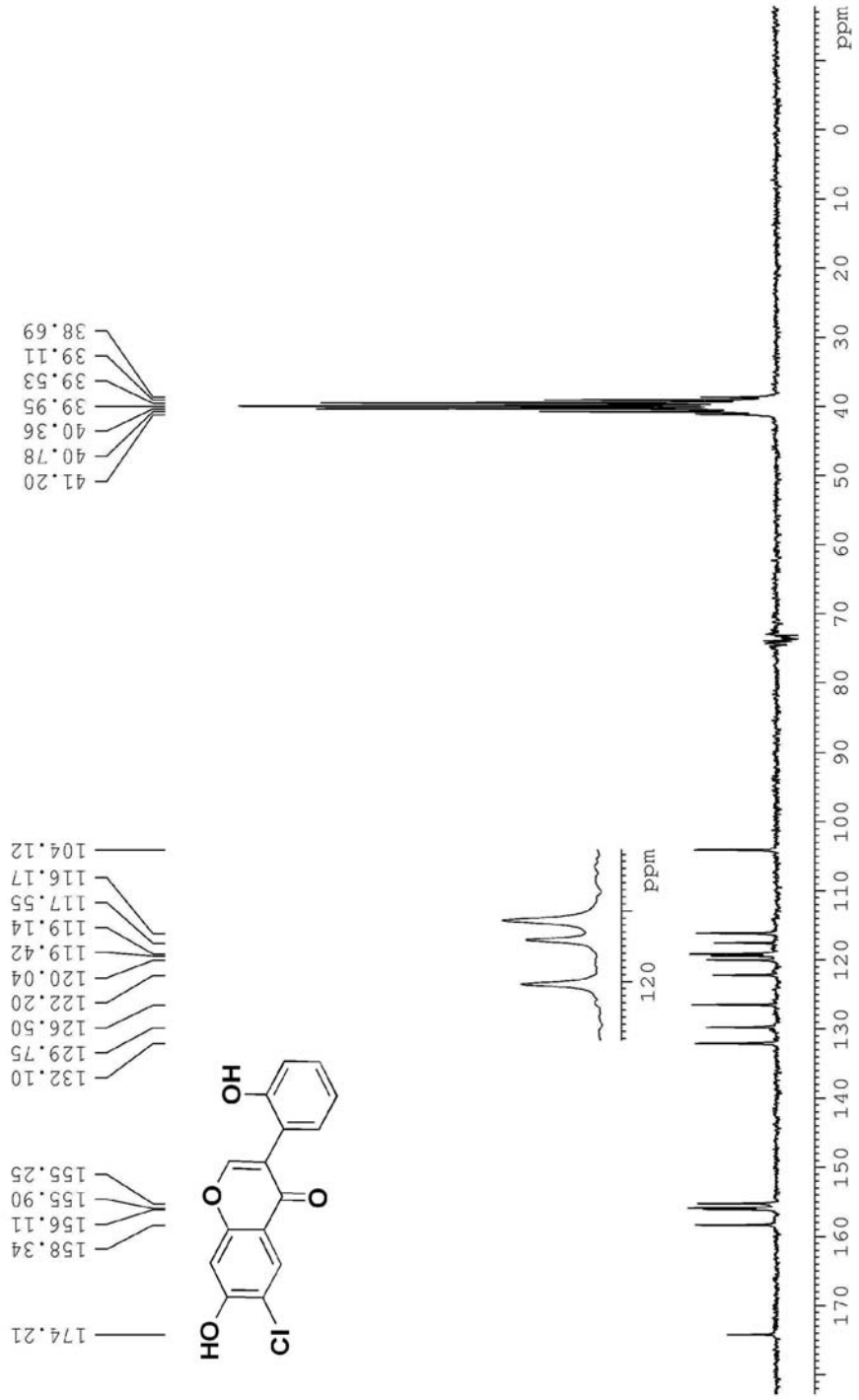

Figure S43. ^{13}C NMR spectrum of **5e** in DMSO-d_6

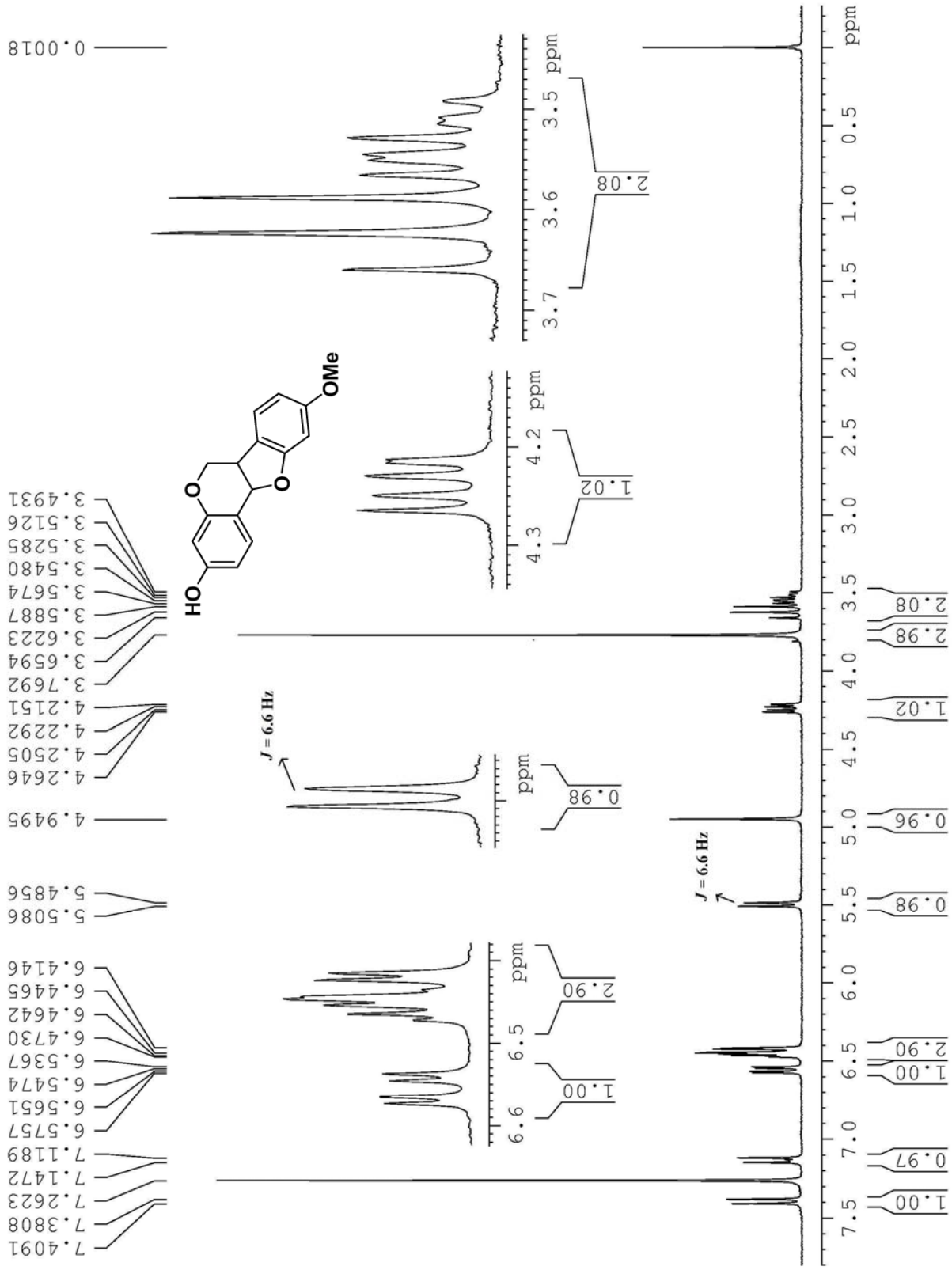

Figure S44. ^{1}H NMR spectrum of **6a** in $CDCl_3$ + DMSO-d_6

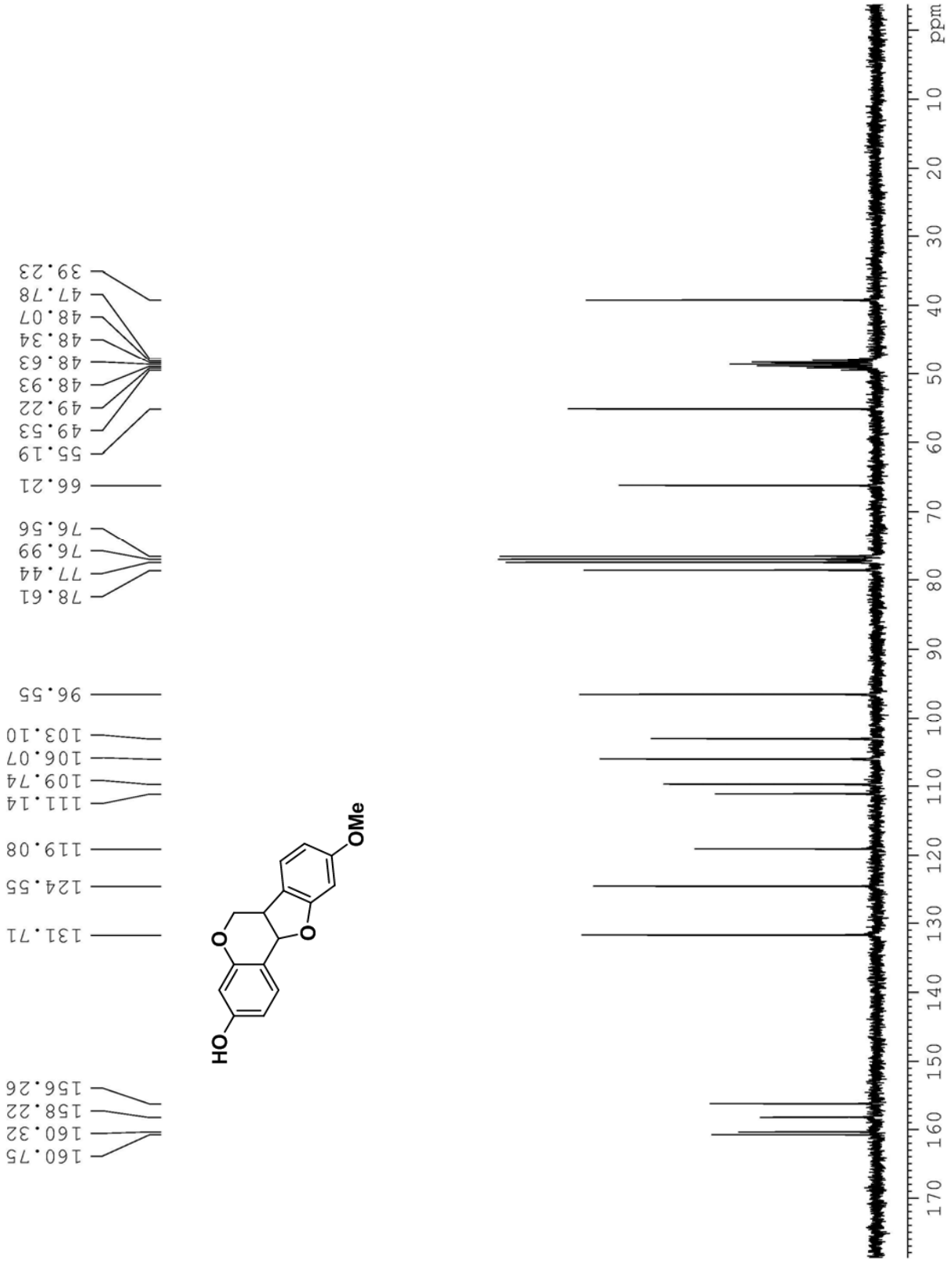

Figure S45. ^{13}C NMR spectrum of **6a** in $CDCl_3$ + DMSO-d_6

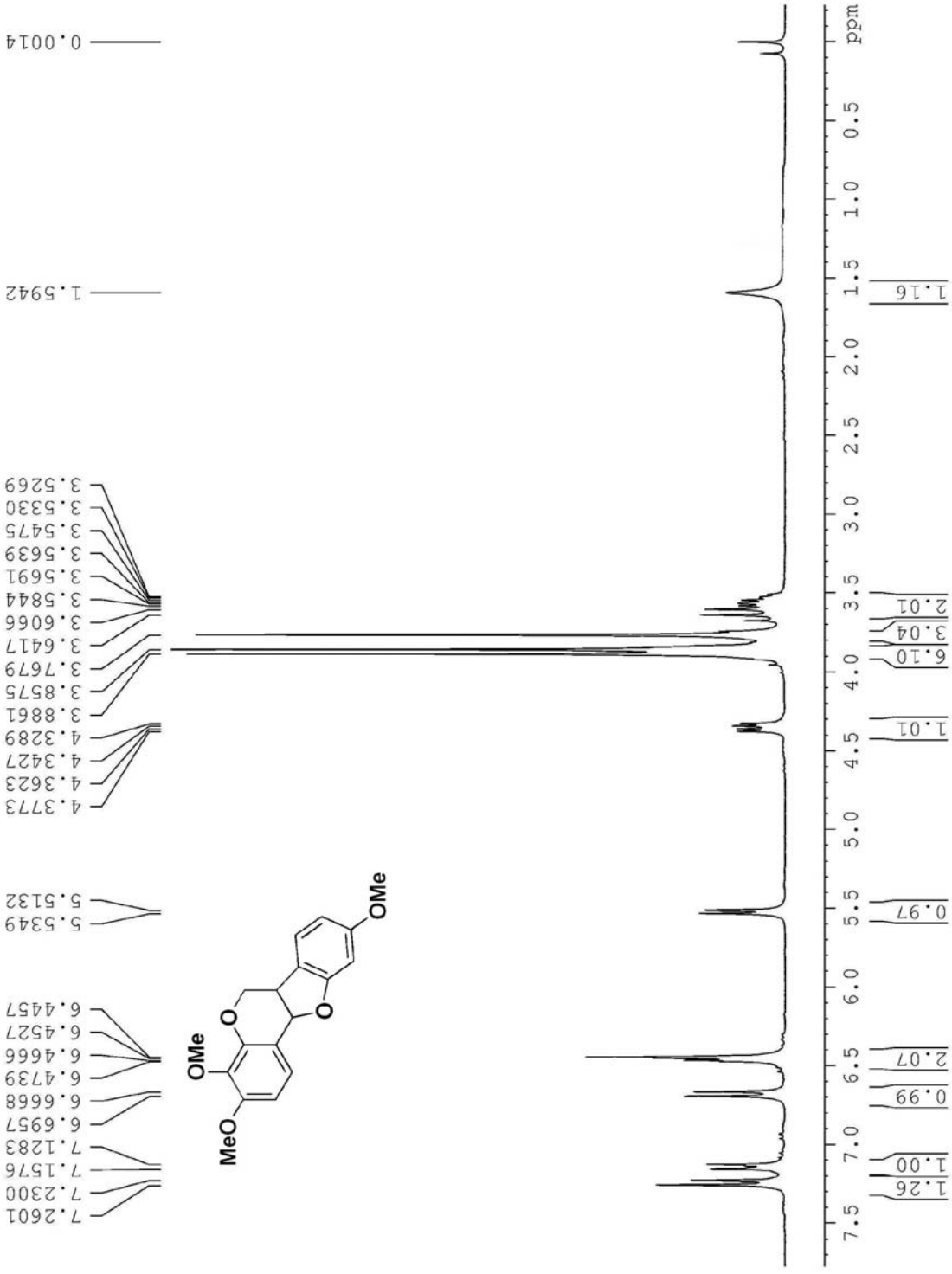

Figure S46. ^{1}H NMR spectrum of **6b** in $CDCl_3$

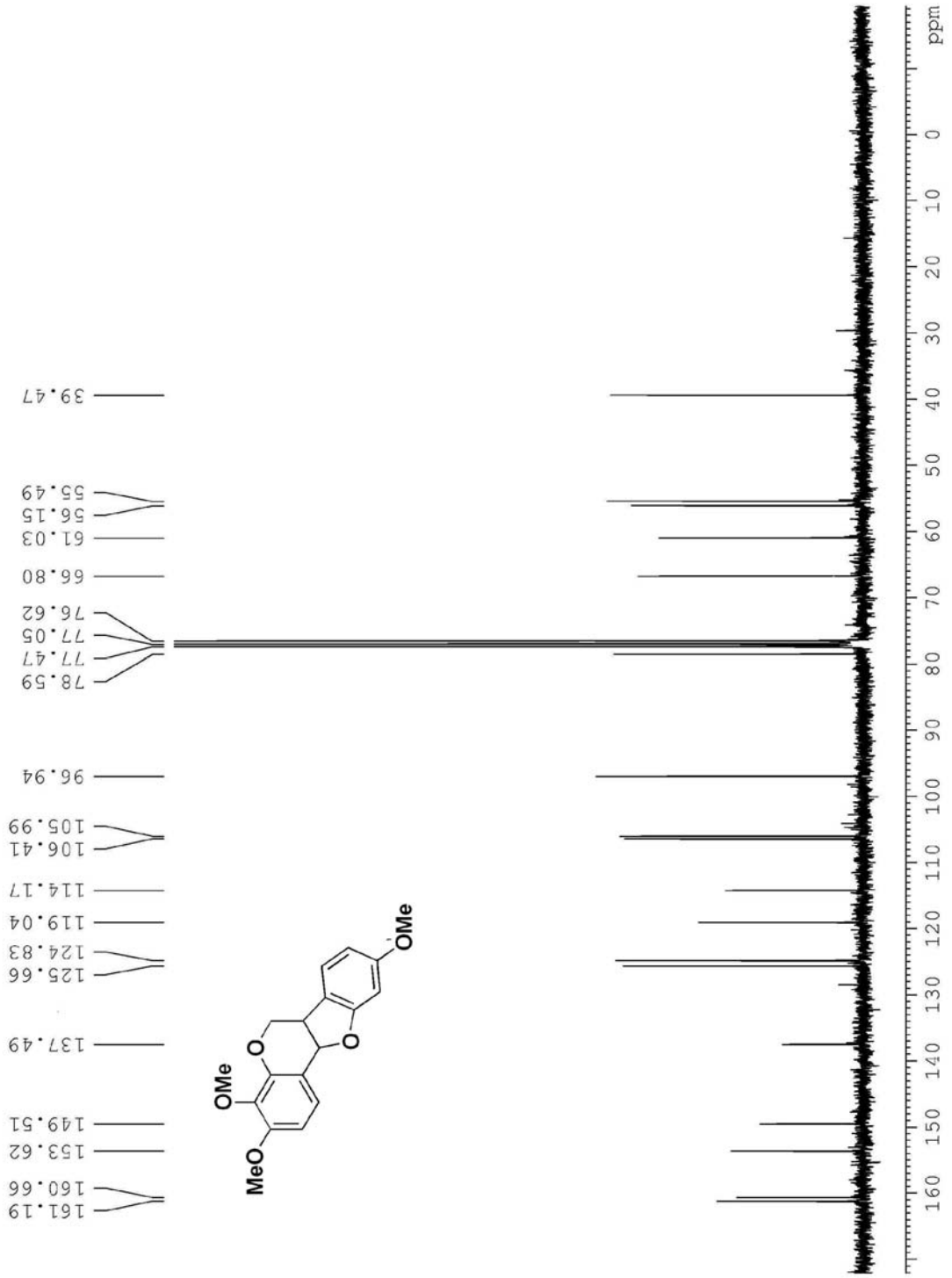

Figure S47. ^{13}C NMR spectrum of **6b** in $CDCl_3$ + DMSO-d_6

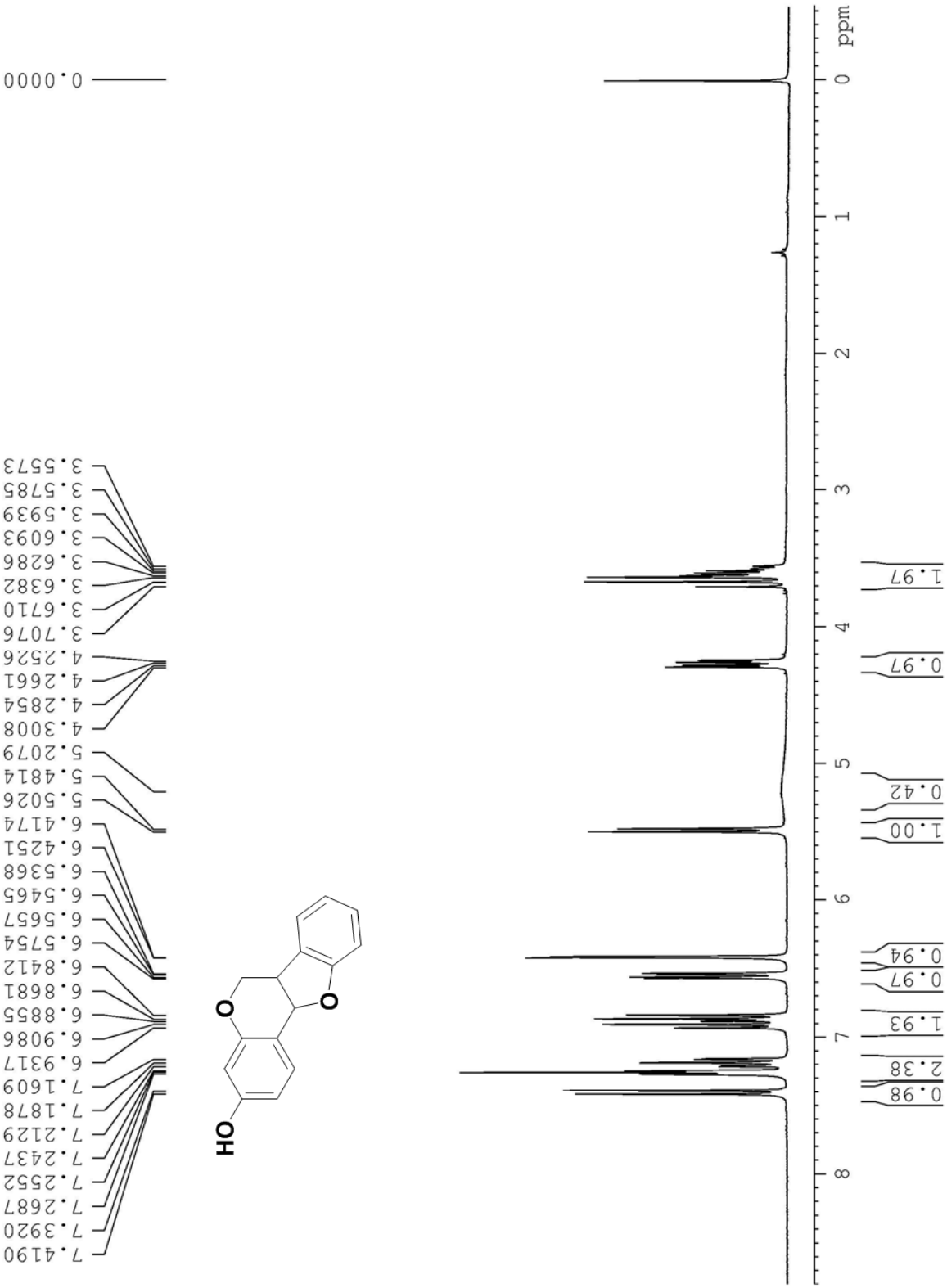

Figure S48. ^{1}H NMR spectrum of **6c** in $CDCl_3$

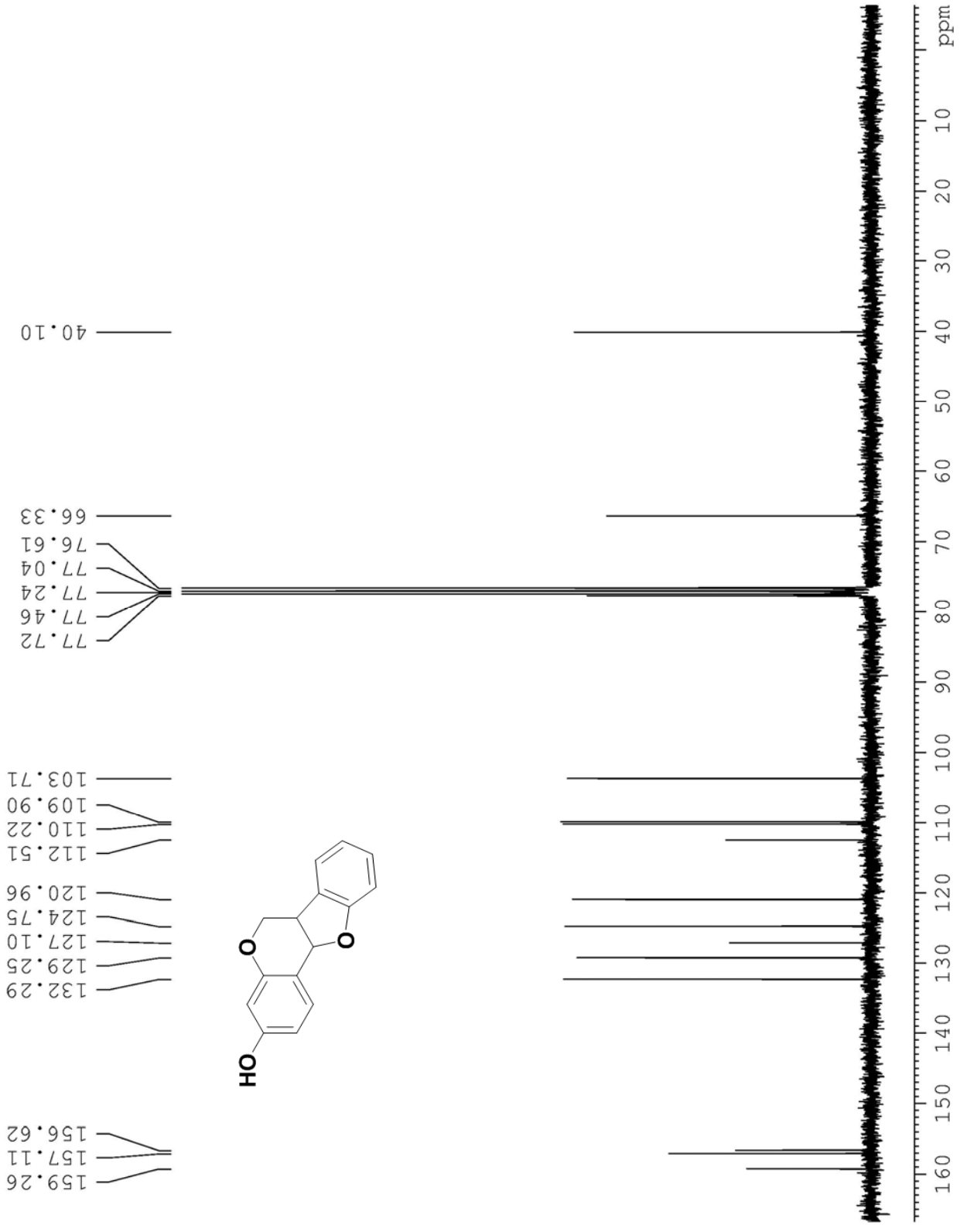

Figure S49. ^{13}C NMR spectrum of **6c** in $CDCl_3$

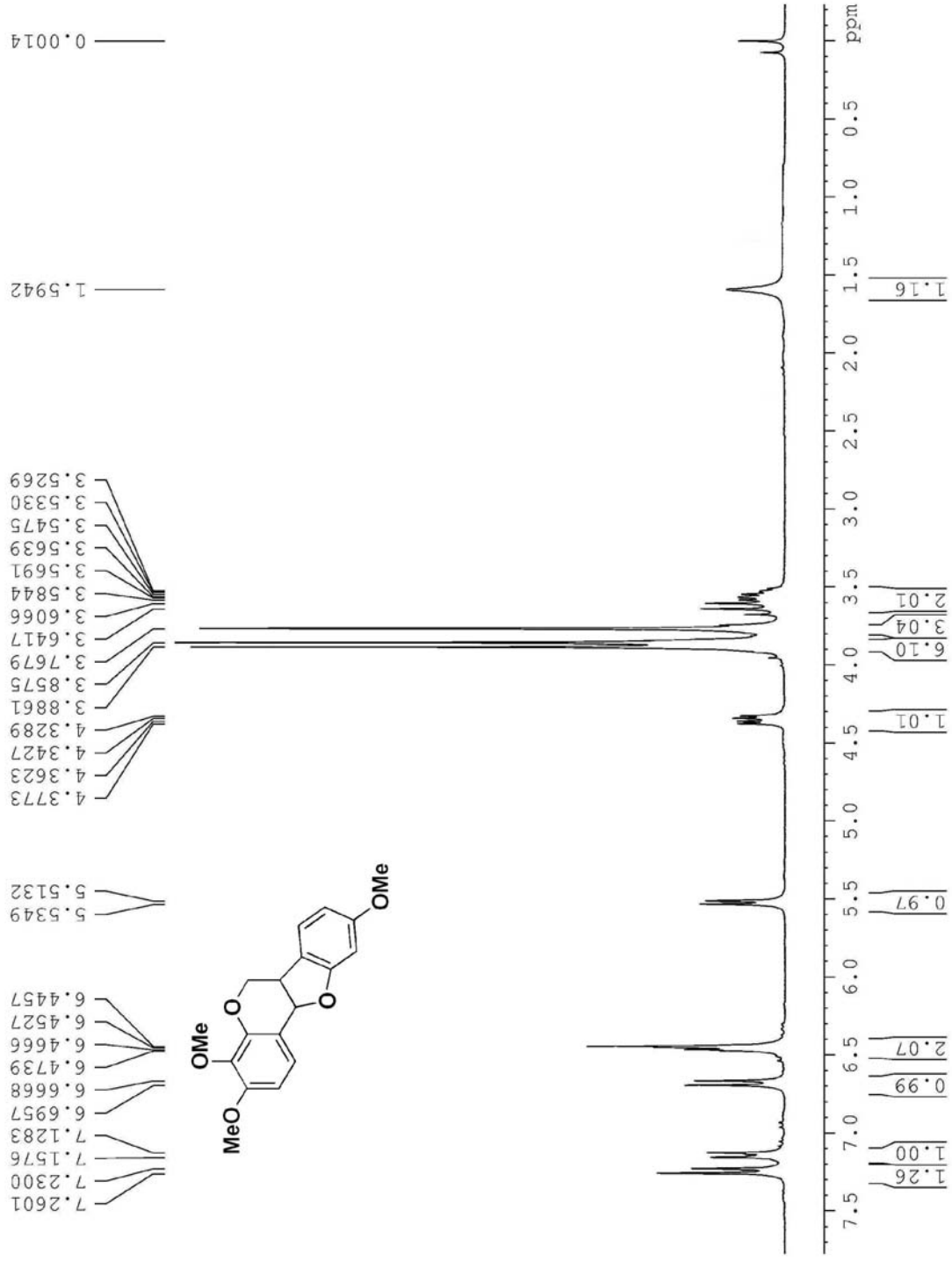

Figure S50. ^{1}H NMR spectrum of **6d** in $CDCl_3$

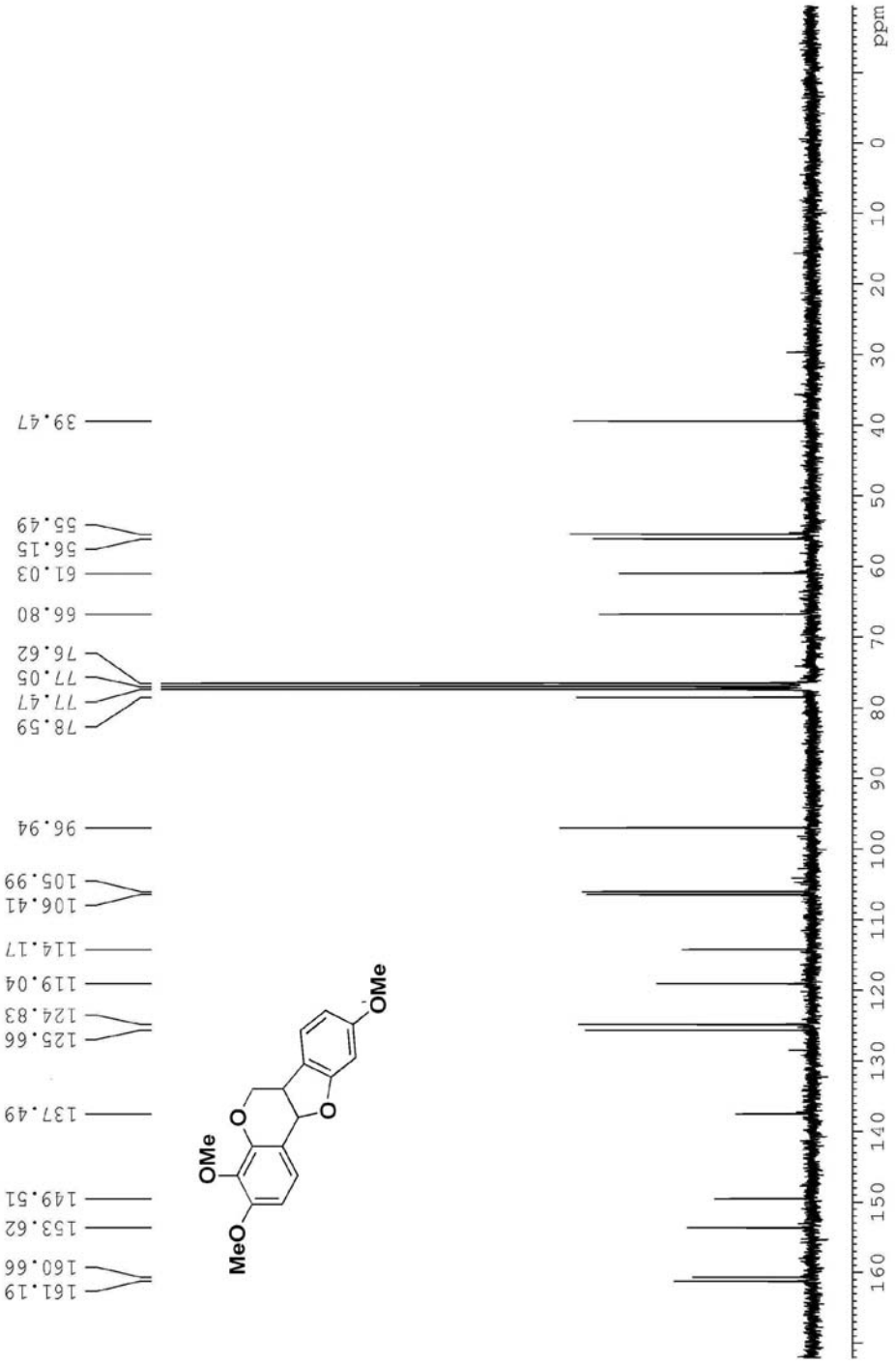

Figure S51. ^{13}C NMR spectrum of **6d** in $CDCl_3$

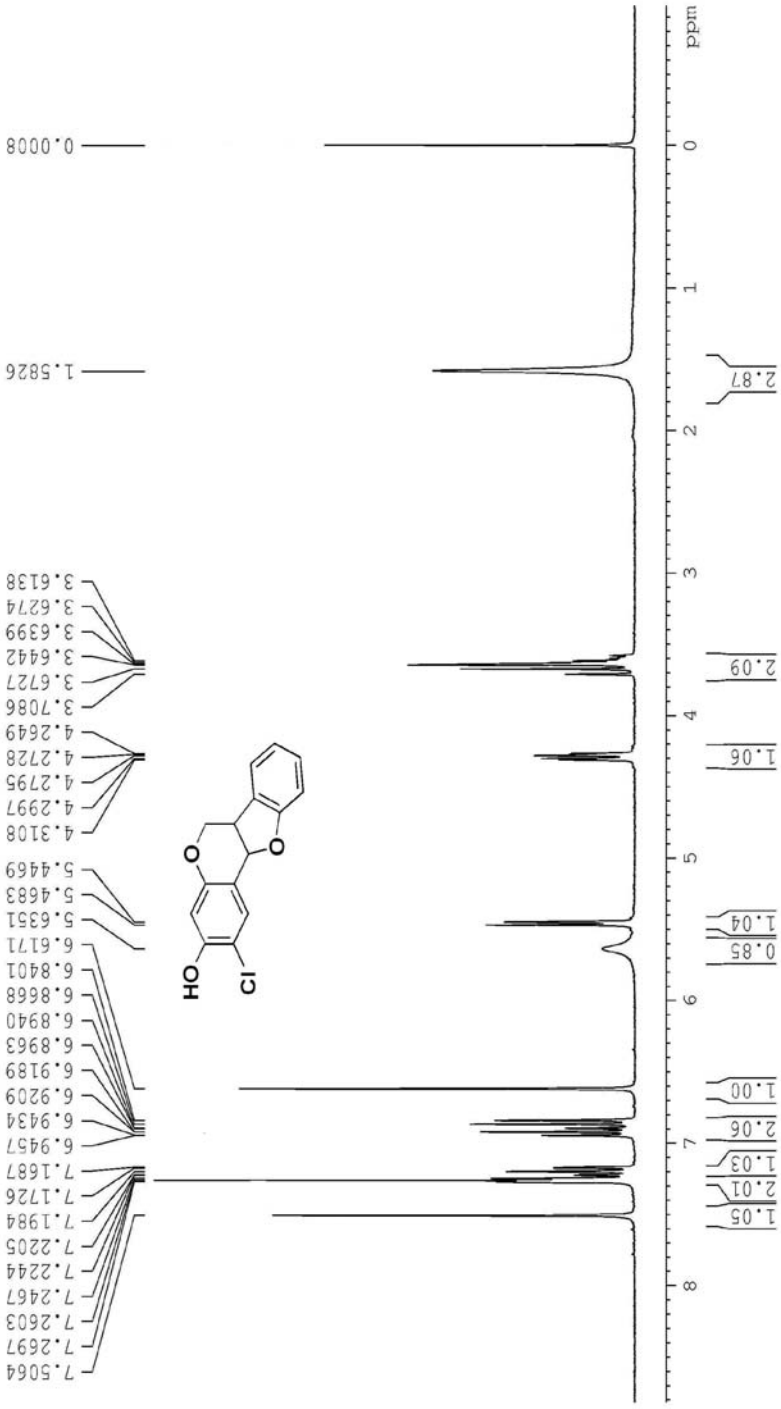

Figure S52. ^{1}H NMR spectrum of **6e** in $CDCl_3$

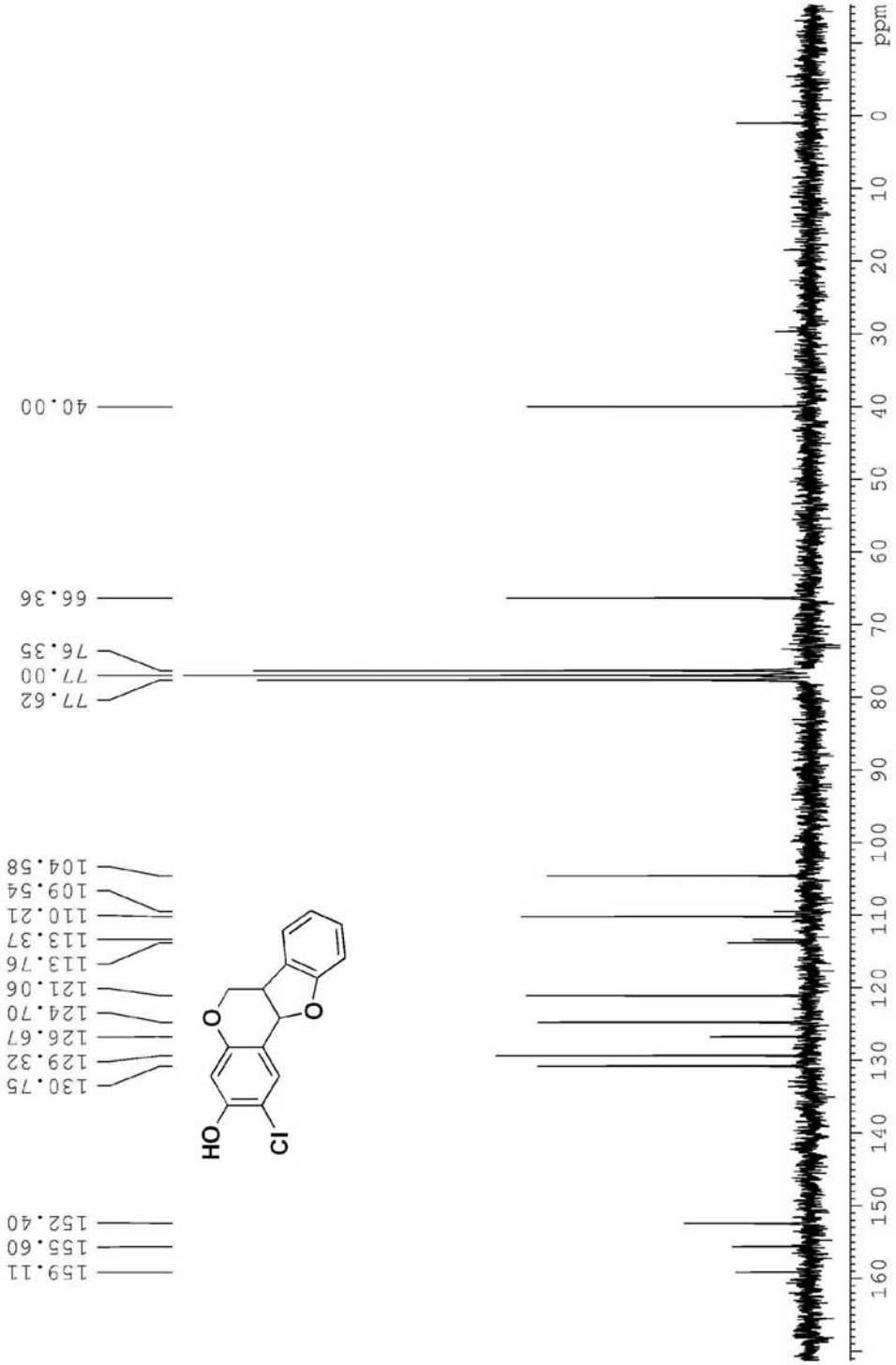

Figure S53. ^{13}C NMR spectrum of **6e** in $CDCl_3$

Cartesian Coordinates and Energies of the B3LYP/6-31G* Optimized Structures of

(6a*R*,11a*R*)-**6a**:

(*R*,*R*)-**6a**$_1$ (H_{anti})

Energy: -919.00281 Hartrees

No imaginary frequency

C	4.173257	-0.230440	0.354893	O	5.533498	-0.138033	0.268555
C	3.632661	-1.492357	0.644757	O	-5.243172	-1.871791	-1.899076
C	2.256184	-1.625375	0.752334	C	-5.060088	-3.171901	-2.436072
C	1.386657	-0.540642	0.562795	H	4.300773	-2.334559	0.788675
C	1.950885	0.706833	0.253468	H	1.830680	-2.596760	0.991752
C	3.337678	0.867273	0.159193	H	3.734575	1.850582	-0.079989
C	-0.092437	-0.680486	0.771880	H	-0.297603	-1.128693	1.753678
C	-0.880903	0.643259	0.633444	H	-0.973304	1.139854	1.605714
C	-0.155656	1.573066	-0.347685	H	-0.637917	2.551693	-0.403855
O	1.193760	1.828315	0.056321	H	-0.151793	1.122285	-1.349486
O	-0.690356	-1.596966	-0.211009	H	-2.711131	-2.876344	-1.466505
C	-1.960011	-1.145340	-0.435723	H	-5.429741	0.438778	-0.916368
C	-2.186688	0.138532	0.064545	H	-3.642380	1.723643	0.264267
C	-2.934268	-1.881010	-1.104215	H	5.774918	0.779665	0.067814
C	-4.189462	-1.274535	-1.268942	H	-4.812275	-3.901663	-1.653856
C	-4.441521	0.015735	-0.771361	H	-4.274182	-3.185476	-3.202790
C	-3.437571	0.723979	-0.111340	H	-6.013799	-3.443519	-2.892494

(*R*,*R*)-**6a**$_2$ (H_{anti})

Energy: -919.002551 Hartrees

No imaginary frequency

C	4.562594	-0.730615	-0.270180	O	5.862714	-0.992432	-0.597904
C	3.852209	-1.740810	0.395718	O	-5.173151	-0.584246	-0.462749
C	2.533166	-1.508795	0.756642	C	-6.349765	0.202389	-0.550503
C	1.882153	-0.301560	0.461228	H	4.350296	-2.676978	0.623483
C	2.607847	0.685228	-0.223972	H	1.980622	-2.280712	1.286466
C	3.944998	0.479212	-0.580837	H	4.472606	1.269676	-1.108521
C	0.486342	-0.031049	0.940341	H	0.411672	-0.221223	2.019806
C	-0.023974	1.395580	0.630605	H	0.203273	2.075448	1.459081
C	0.642384	1.912284	-0.651120	H	0.369311	2.950353	-0.854247
O	2.070132	1.899093	-0.552815	H	0.334501	1.291886	-1.503887
O	-0.483725	-0.938591	0.311469	H	-2.997784	-1.881385	-0.247391
C	-1.655091	-0.243876	0.208200	H	-4.724892	2.074198	-0.013916
C	-1.497891	1.133594	0.426131	H	-2.510099	3.034913	0.496820
C	-2.880001	-0.815862	-0.087845	H	6.236054	-0.218468	-1.047700
C	-3.993521	0.039741	-0.171695	H	-6.276374	0.953120	-1.348580
C	-3.864057	1.419553	0.043513	H	-6.570388	0.707434	0.399274
C	-2.603806	1.963341	0.337046	H	-7.157430	-0.493790	-0.784446

(*R*,*R*)-**6a**$_3$ (H_{anti})

Energy: -919.0024266 Hartrees

No imaginary frequency

C	4.573963	-0.624800	-0.300306	O	5.868175	-0.947417	-0.596853
C	4.017984	0.622277	-0.623817	O	-3.444292	2.297956	4.554579
C	2.690146	0.876015	-0.301863	C	-3.036663	3.642049	4.751412
C	1.895973	-0.072125	0.353821	H	4.617670	1.375484	-1.130489
C	2.483630	-1.306696	0.686046	H	2.250029	1.834666	-0.564780
C	3.810226	-1.589228	0.353655	H	4.242263	-2.548127	0.616288
C	0.440142	0.179608	0.616569	H	-0.067775	0.482108	-0.309421
C	-0.307262	-1.018230	1.248377	H	-0.744970	-1.652831	0.469843
C	0.670737	-1.846854	2.091096	H	0.196817	-2.749824	2.482822
O	1.788614	-2.298352	1.320553	H	1.034277	-1.244172	2.934657
O	0.249108	1.298434	1.552428	H	-1.171639	2.959973	3.139299
C	-0.885734	1.018720	2.259994	H	-4.046359	-0.110536	4.134589
C	-1.320300	-0.299680	2.109090	H	-2.819543	-1.742021	2.694772
C	-1.544502	1.946711	3.061381	H	6.288934	-0.188581	-1.029965
C	-2.692393	1.503950	3.737207	H	-3.039854	4.207973	3.810334
C	-3.150131	0.182192	3.598253	H	-2.037013	3.699366	5.202124
C	-2.459506	-0.720454	2.789942	H	-3.766355	4.078426	5.436094

(*R*,*R*)-**6a**$_4$ (H_{anti})

Energy: -919.0022154 Hartrees

No imaginary frequency

C	4.676133	-0.429783	-0.330399	C	0.488946	0.018214	0.586935
C	4.036712	0.795872	-0.570893	C	-0.178234	-1.272666	1.115773
C	2.691937	0.933212	-0.248399	C	0.846601	-2.090599	1.912449
C	1.961075	-0.112733	0.326888	O	2.001259	-2.405690	1.128985
C	2.630983	-1.324453	0.577283	O	0.212694	1.045703	1.601107
C	3.976660	-1.489586	0.242956	C	-0.909706	0.642501	2.266810

C	-1.250020	-0.694609	2.010228	H	-0.029494	0.353787	-0.321702
C	-1.646246	1.448354	3.117274	H	-0.560498	-1.877376	0.286064
C	-2.772456	0.879060	3.739061	H	0.433118	-3.050648	2.229784
C	-3.135410	-0.454040	3.498431	H	1.157366	-1.527835	2.803396
C	-2.360442	-1.241441	2.632622	H	-1.383933	2.482856	3.306168
O	5.991839	-0.639980	-0.633547	H	-4.007633	-0.886854	3.972621
O	-3.459374	1.724755	4.562660	H	-2.644571	-2.276064	2.455637
C	-4.616949	1.235454	5.219342	H	6.361698	0.176262	-1.004159
H	4.585870	1.623676	-1.014435	H	-4.379790	0.395610	5.885886
H	2.187775	1.875531	-0.447362	H	-5.385738	0.919171	4.501874
H	4.472817	-2.432718	0.441589	H	-4.998610	2.068834	5.812238

(*R*,*R*)-**6a**$_5$ (O_{anti})

Energy: -918.999822 Hartrees

No imaginary frequency

C	3.527362	-0.175690	-0.575612	C	-2.674131	-1.669512	-0.815320
C	3.208113	-1.302005	0.197062	C	-3.591946	-0.969538	-1.612717
C	2.006052	-1.323317	0.889520	C	-3.731102	0.424826	-1.500883
C	1.100179	-0.252913	0.845917	C	-2.958720	1.136953	-0.584212
C	1.451662	0.867552	0.080240	O	4.718033	-0.191992	-1.245291
C	2.656880	0.910995	-0.628733	O	-4.399069	-1.564139	-2.540267
C	-0.244058	-0.359978	1.528495	C	-4.312801	-2.969968	-2.704738
C	-1.121189	0.910070	1.328568	H	3.902309	-2.134671	0.232382
C	-0.267173	2.146608	1.057228	H	1.741588	-2.204291	1.469166
O	0.648768	1.970543	-0.022332	H	2.891366	1.802436	-1.204977
O	-1.004449	-1.467595	0.937628	H	-0.127254	-0.628545	2.581936
C	-1.919804	-0.920749	0.083653	H	-1.698839	1.113244	2.242993
C	-2.040812	0.460405	0.213801	H	0.296126	2.416520	1.963507

H	-0.890431	2.999070	0.774800	H	4.808222	0.633140	-1.747068
H	-2.534756	-2.740915	-0.881597	H	-4.569878	-3.501814	-1.779014
H	-4.450380	0.923269	-2.141794	H	-3.310333	-3.278705	-3.029694
H	-3.080265	2.214684	-0.504751	H	-5.037421	-3.225561	-3.480233

(*R*,*R*)-**6a**$_6$ (O_{anti})

Energy: -918.9994542 Hartrees

No imaginary frequency

C	3.708382	-1.015383	-0.867394	O	4.673910	-1.577004	-1.654138
C	3.377538	-1.684140	0.320326	O	-4.481873	-1.023633	-0.771802
C	2.400206	-1.146161	1.144850	C	-5.459405	-0.508542	-1.659844
C	1.734126	0.048148	0.831416	H	3.885844	-2.610172	0.566463
C	2.095546	0.705292	-0.353059	H	2.120744	-1.673569	2.053489
C	3.076229	0.180538	-1.201674	H	3.329183	0.725740	-2.107457
C	0.605783	0.545978	1.705359	H	0.929787	0.641389	2.745315
C	-0.041951	1.850507	1.159697	H	-0.339413	2.498016	1.998173
C	0.936512	2.648992	0.302252	H	1.740578	3.054760	0.934993
O	1.517377	1.880494	-0.749921	H	0.434057	3.485267	-0.190919
O	-0.469193	-0.450958	1.734083	H	-2.641625	-1.827085	0.791268
C	-1.444944	-0.023649	0.878964	H	-4.009764	1.565064	-1.512485
C	-1.267792	1.300666	0.462237	H	-2.088042	2.895750	-0.733989
C	-2.515235	-0.799943	0.469446	H	4.796764	-1.026794	-2.443356
C	-3.448852	-0.209916	-0.400704	H	-5.019154	-0.221624	-2.624085
C	-3.293195	1.113821	-0.837234	H	-5.979957	0.357968	-1.230597
C	-2.196364	1.868280	-0.394188	H	-6.175819	-1.317125	-1.817302

(*R*,*R*)-**6a**$_7$ (O_{anti})

Energy: -918.999375 Hartrees

No imaginary frequency

C	3.760433	-1.169567	-0.650738	O	4.756732	-1.907085	-1.226131
C	3.141426	-0.097477	-1.310501	O	3.456482	4.690774	5.215132
C	2.135026	0.607717	-0.660729	C	3.890248	5.781479	4.419790
C	1.716726	0.277119	0.633338	H	3.451050	0.181018	-2.315628
C	2.342406	-0.811731	1.264222	H	1.671692	1.455490	-1.159297
C	3.357299	-1.532828	0.632361	H	3.821536	-2.371305	1.138969
C	0.693098	1.131236	1.346286	H	-0.210392	1.243968	0.740828
C	0.387881	0.626265	2.786256	H	-0.679462	0.768363	3.013664
C	0.680557	-0.865522	2.932466	H	-0.046175	-1.446977	2.344738
O	1.999462	-1.221419	2.523392	H	0.604470	-1.178984	3.976901
O	1.216638	2.493399	1.502186	H	2.682284	4.487181	2.574947
C	1.639328	2.619812	2.795416	H	2.622027	2.695582	6.508089
C	1.232632	1.569989	3.614754	H	1.274825	0.788118	5.629903
C	2.385646	3.700512	3.256783	H	4.934380	-1.555368	-2.112181
C	2.727236	3.702512	4.617503	H	3.042188	6.329958	3.988537
C	2.330009	2.653213	5.464305	H	4.554568	5.452677	3.609540
C	1.579177	1.590937	4.962555	H	4.441744	6.441534	5.092104

(*R*,*R*)-**6a**$_8$ (O_{anti})

Energy: -918.9991372 Hartrees

No imaginary frequency

C	3.814259	-1.171101	-0.617979	C	3.100713	-0.251621	-1.400970

C	2.101304	0.511019	-0.808242	O	3.607491	5.637474	3.932202
C	1.781896	0.385596	0.548698	C	4.117329	5.954576	5.216411
C	2.501168	-0.554884	1.305920	H	3.333360	-0.133349	-2.457239
C	3.511249	-1.329779	0.732565	H	1.564916	1.243879	-1.405738
C	0.758726	1.303136	1.178955	H	4.050052	-2.050687	1.336850
C	0.585680	1.047875	2.703107	H	-0.189724	1.261487	0.636425
C	0.958140	-0.384021	3.079244	H	-0.466966	1.193966	2.988395
O	2.260703	-0.759514	2.637239	H	0.220403	-1.083519	2.657176
O	1.204570	2.694532	1.055249	H	0.969983	-0.513837	4.164615
C	1.725529	3.064600	2.262970	H	2.665405	4.926551	1.677922
C	1.443738	2.150948	3.284924	H	2.995012	3.766325	5.828828
C	2.445543	4.227285	2.476218	H	1.694949	1.721806	5.382651
C	2.901624	4.477082	3.782583	H	4.916314	-1.743793	-2.073515
C	2.637320	3.576138	4.824376	H	4.824708	5.192873	5.570326
C	1.898892	2.411315	4.566698	H	3.312460	6.068156	5.954886
O	4.810097	-1.952911	-1.132580	H	4.639545	6.906680	5.103898

Cartesian Coordinates and Energies of the B3LYP/6-31G* Optimized Structures of (6a*R*,11a*R*)-**6c**:

(*R*,*R*)-**6c**$_1$ (H_{anti})
Energy: -804.480123 Hartrees
No imaginary frequency

C	-4.519092	-0.898241	2.839274	C	-4.069032	-1.769407	1.835528

C	-2.744919	-1.699603	1.428585	C	3.032753	0.408904	2.351502
C	-1.837151	-0.795990	2.001524	O	-5.832227	-0.990001	3.203802
C	-2.306641	0.050283	3.017775	H	-4.766343	-2.471817	1.391976
C	-3.642845	0.009557	3.430619	H	-2.392567	-2.361188	0.641156
C	-0.433549	-0.669197	1.487282	H	-3.966774	0.684158	4.218997
C	0.385049	0.460663	2.154296	H	-0.439474	-0.524979	0.398095
C	-0.108121	0.673829	3.591737	H	0.286581	1.395505	1.592075
O	-1.506631	0.971923	3.635771	H	0.390886	1.522622	4.064888
O	0.338114	-1.898373	1.718731	H	0.086958	-0.228508	4.187164
C	1.634990	-1.511689	1.909992	H	2.595801	-3.434965	1.729426
C	1.774292	-0.135585	2.128155	H	4.863339	-2.457643	2.124480
C	2.726969	-2.372216	1.904794	H	5.141161	-0.027892	2.506760
C	3.989984	-1.810742	2.127967	H	3.154249	1.475671	2.524370
C	4.149142	-0.438899	2.344018	H	-6.013503	-0.337679	3.898362

(*R*,*R*)-**6c**$_2$ (H$_{anti}$)

Energy: -804.479775 Hartrees

No imaginary frequency

C	3.985837	-0.243242	-0.198017	C	-0.930874	0.901427	0.737941
C	3.427030	-1.466491	0.202733	C	-0.302080	1.767095	-0.362227
C	2.071274	-1.526472	0.501931	O	1.099016	1.959258	-0.151277
C	1.242638	-0.403106	0.397484	O	-0.970515	-1.361540	-0.058866
C	1.823578	0.806088	-0.026387	C	-2.236509	-0.850108	-0.122313
C	3.187297	0.892659	-0.313169	C	-2.327955	0.459121	0.365719
C	-0.199484	-0.459133	0.808090	C	-3.340981	-1.529697	-0.623493

C	-4.566835	-0.853231	-0.624903	H	-0.866471	1.426836	1.696843
C	-4.678322	0.452502	-0.138599	H	-0.738826	2.768151	-0.382598
C	-3.549548	1.120642	0.356021	H	-0.458644	1.293120	-1.340900
O	5.312030	-0.107628	-0.496620	H	-3.247442	-2.545676	-0.992900
H	4.051310	-2.353409	0.287656	H	-5.449326	-1.360506	-1.005836
H	1.636827	-2.468236	0.827676	H	-5.642796	0.951765	-0.143956
H	3.614813	1.835486	-0.634726	H	-3.633540	2.138358	0.729896
H	-0.290794	-0.873974	1.821382	H	5.746399	-0.968449	-0.392942

(*R*,*R*)-**6c**$_3$ (O_{anti})

Energy: -804.477146 Hartrees

No imaginary frequency

C	3.385118	-0.197056	-1.240009	C	-2.989544	0.082112	-0.920293
C	2.797454	-1.453372	-1.030268	C	-3.697506	1.275392	-1.103387
C	1.685119	-1.546323	-0.206540	C	-3.412775	2.412964	-0.342260
C	1.130492	-0.424446	0.427689	C	-2.407793	2.375501	0.633581
C	1.747280	0.816395	0.214619	O	4.476940	-0.145322	-2.059286
C	2.868149	0.935295	-0.613651	H	3.218552	-2.324247	-1.520925
C	-0.142455	-0.551403	1.233036	H	1.209711	-2.513218	-0.061354
C	-0.620512	0.809360	1.815499	H	3.318021	1.915953	-0.746169
C	0.537464	1.789091	1.985978	H	-0.044350	-1.324595	1.999866
O	1.294641	1.972366	0.791303	H	-1.064848	0.655687	2.810006
O	-1.228573	-1.015270	0.363729	H	1.207732	1.437984	2.785204
C	-1.994282	0.072680	0.050528	H	0.173568	2.783801	2.256398
C	-1.697609	1.197185	0.823508	H	-3.197949	-0.804302	-1.510352

H	-4.479463	1.315899	-1.857134	H	-2.190499	3.259765	1.228469
H	-3.972262	3.329161	-0.506919	H	4.773756	0.775235	-2.131321

(*R*,*R*)-**6c**$_4$ (O_{anti})

Energy: -804.476777 Hartrees

No imaginary frequency

C	3.464559	-0.326812	-0.684567
C	3.172717	-1.332338	0.249051
C	1.999005	-1.249937	0.989145
C	1.099392	-0.189110	0.833394
C	1.424461	0.812556	-0.097609
C	2.596229	0.749643	-0.853520
C	-0.214748	-0.185488	1.581682
C	-1.096507	1.047571	1.235271
C	-0.253649	2.227683	0.759188
O	0.615159	1.893431	-0.320374
O	-1.003380	-1.359522	1.195133
C	-1.949612	-0.938905	0.302270
C	-2.061143	0.451220	0.230995
C	-2.748983	-1.786757	-0.455932
C	-3.685536	-1.193518	-1.310214

C	-3.809439	0.196101	-1.399066
C	-2.994870	1.028457	-0.619746
O	4.597925	-0.342449	-1.447567
H	3.854175	-2.169407	0.385692
H	1.757002	-2.041448	1.694008
H	2.826427	1.536511	-1.562784
H	-0.051901	-0.295550	2.657278
H	-1.644823	1.378762	2.129582
H	0.345653	2.618475	1.595608
H	-0.886680	3.036527	0.384979
H	-2.639889	-2.863976	-0.384715
H	-4.322931	-1.829192	-1.919209
H	-4.539389	0.633000	-2.074214
H	-3.095355	2.109372	-0.686500
H	5.109468	-1.137452	-1.231494