

Computationally Assisted Structural Elucidation of Cembranoids from the Soft Coral *Sarcophyton tortuosum*

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Figure S1. LR- and HR-ESIMS spectra of **1**.

Figure S2. ^1H NMR spectrum of **1** in CDCl_3 .

Figure S3. ^{13}C NMR spectrum of **1** in CDCl_3 .

Figure S4. DEPT and ^{13}C NMR spectra of **1** in CDCl_3 .

Figure S5. HSQC spectrum of **1** in CDCl_3 .

Figure S6. ^1H - ^1H COSY spectrum of **1** in CDCl_3 .

Figure S7. HMBC spectrum of **1** in CDCl_3 .

Figure S8. NOESY spectrum of **1** in CDCl_3 .

Figure S9. LR- and HR-ESIMS spectra of **2**.

Figure S10. ^1H NMR spectrum of **2** in CDCl_3 .

Figure S11. ^{13}C NMR spectrum of **2** in CDCl_3 .

Figure S12. DEPT and ^{13}C NMR spectra of **2** in CDCl_3 .

Figure S13. HSQC spectrum of **2** in CDCl_3 .

Figure S14. ^1H - ^1H COSY spectrum of **2** in CDCl_3 .

Figure S15. HMBC spectrum of **2** in CDCl_3 .

Figure S16. NOESY spectrum of **2** in CDCl_3 .

Figure S17. LR- and HR-ESIMS spectra of **3**.

Figure S18. ^1H NMR spectrum of **3** in CDCl_3 .

Figure S19. ^{13}C NMR spectrum of **3** in CDCl_3 .

Figure S20. DEPT and ^{13}C NMR spectra of **3** in CDCl_3 .

Figure S21. HSQC spectrum of **3** in CDCl_3 .

Figure S22. ^1H - ^1H COSY spectrum of **3** in CDCl_3 .

Figure S23. HMBC spectrum of **3** in CDCl_3 .

Figure S24. NOESY spectrum of **3** in CDCl_3 .

Table S1. Low-energy conformers of **1R,2S,7S,8R-1** for ECD calculations.

Table S2. Low-energy conformers of **2** for ECD calculations.

Table S3. Conformers of **1R*,2S*,7S*,8S*-1** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

Table S4. Conformers of **1R*,2S*,7R*,8S*-1** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

Table S5. Conformers of **1R*,2S*,7S*,8R*-1** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

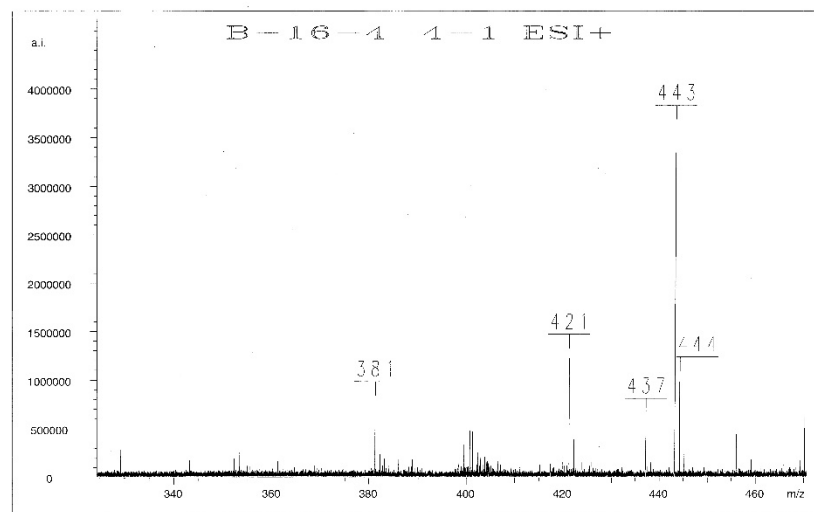
Table S6. Conformers of **1R*,2S*,7R*,8R*-1** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

Table S7. Conformers of 1*R**,2*R**,7*R**,8*R**-**2** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

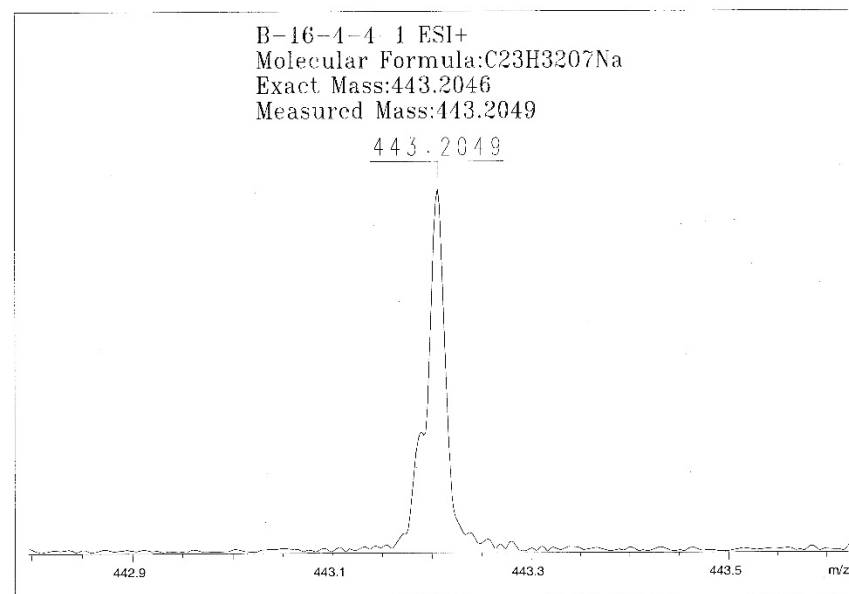
Table S8. Conformers of 1*R**,2*R**,7*S**,8*R**-**2** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

Table S9. Conformers of 1*R**,2*R**,7*R**,8*S**-**2** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

Table S10. Conformers of 1*R**,2*R**,7*S**,8*S**-**2** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (none of the conformers was selected).



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Figure S1. LR- and HR-ESIMS spectra of **1**.

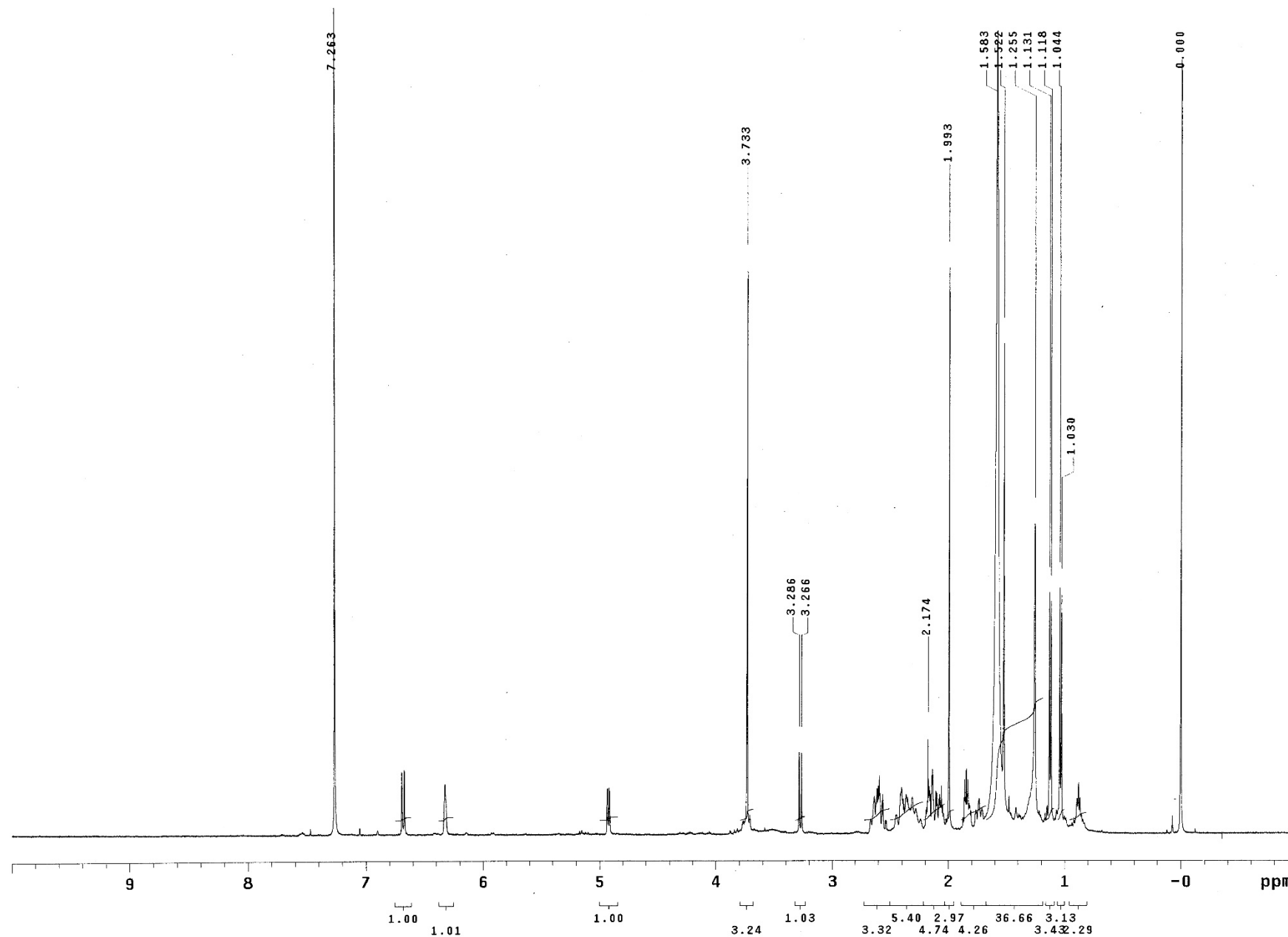


Figure S2. ¹H NMR spectrum of **1** in CDCl₃.

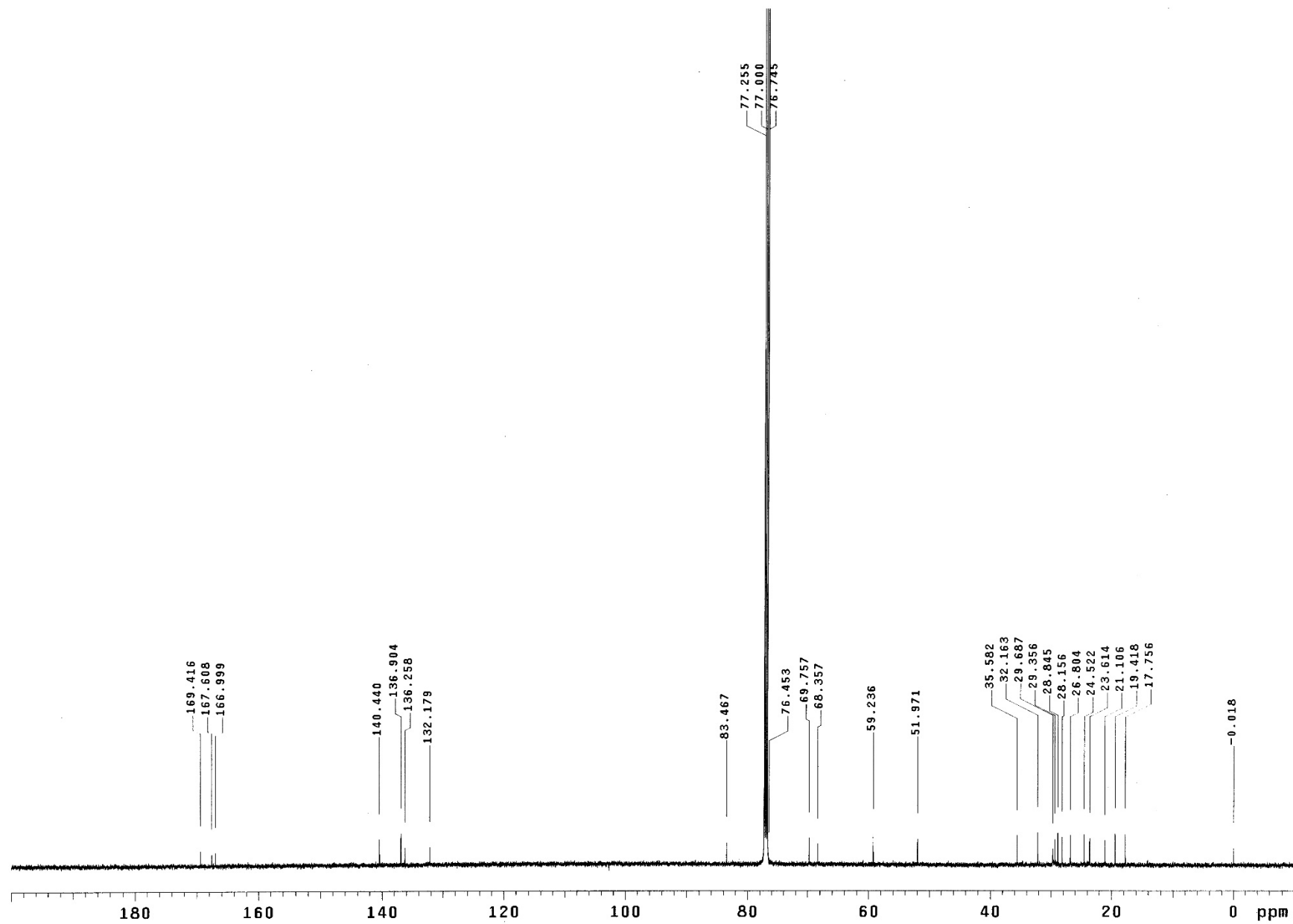


Figure S3. ¹³C NMR spectrum of **1** in CDCl₃.

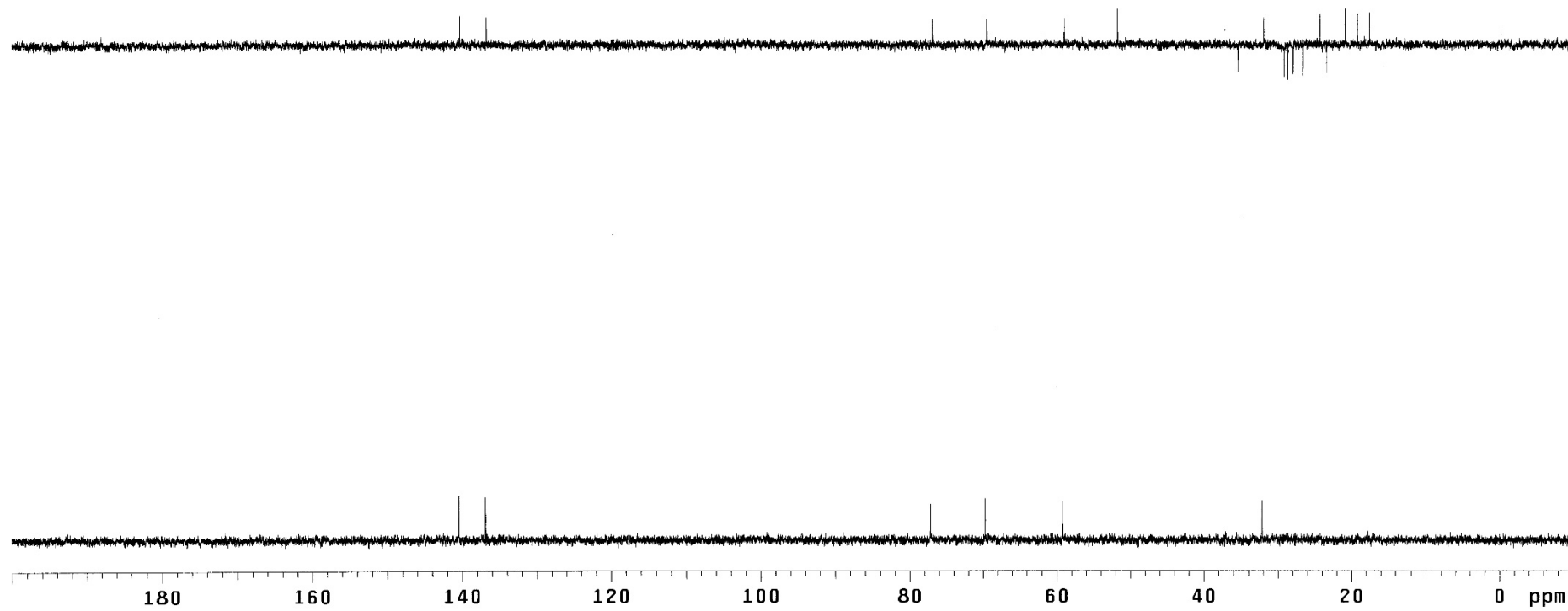


Figure S4. DEPT and ^{13}C NMR spectra of **1** in CDCl_3 .

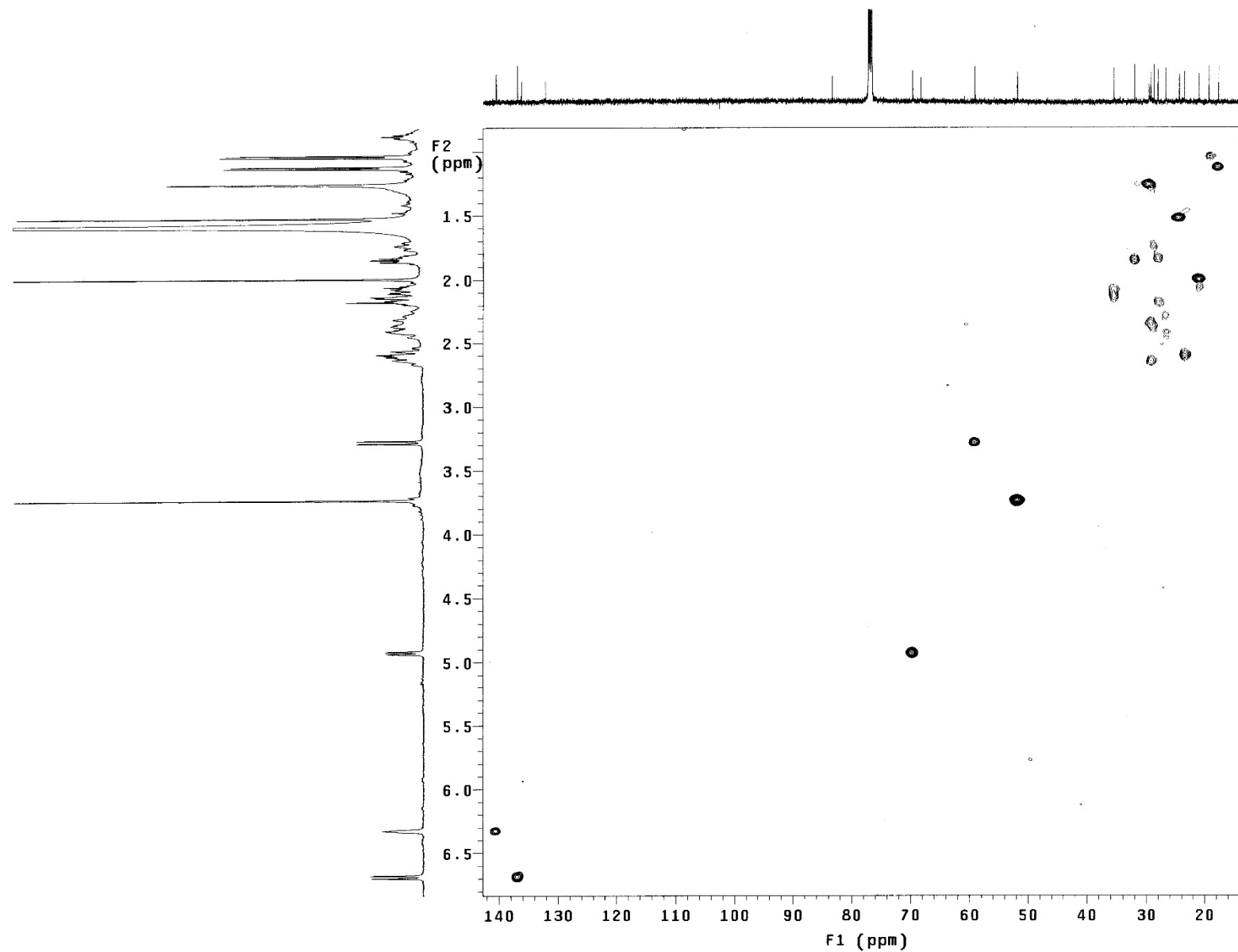


Figure S5. HSQC spectrum of **1** in CDCl₃.

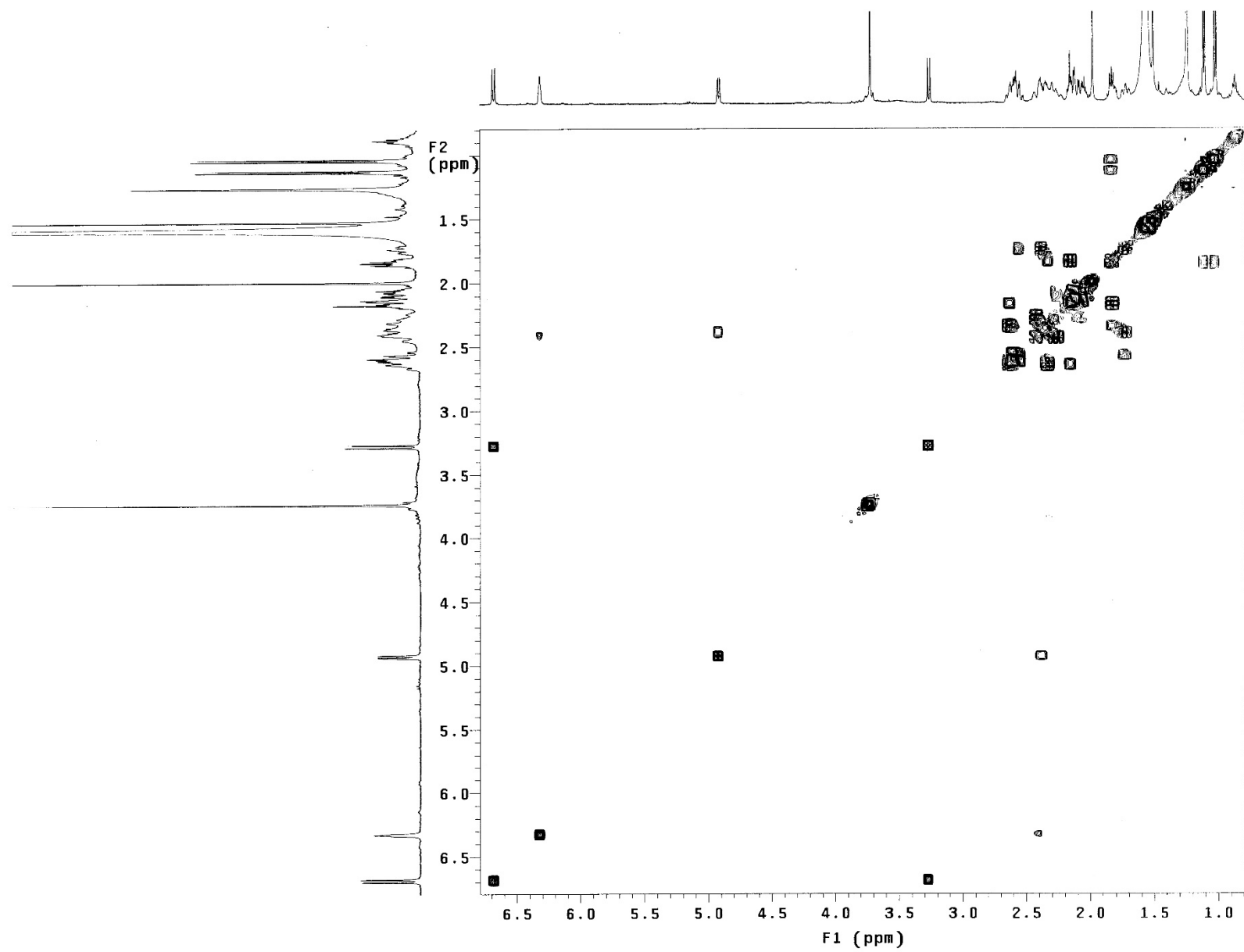


Figure S6. ^1H - ^1H COSY spectrum of **1** in CDCl_3 .

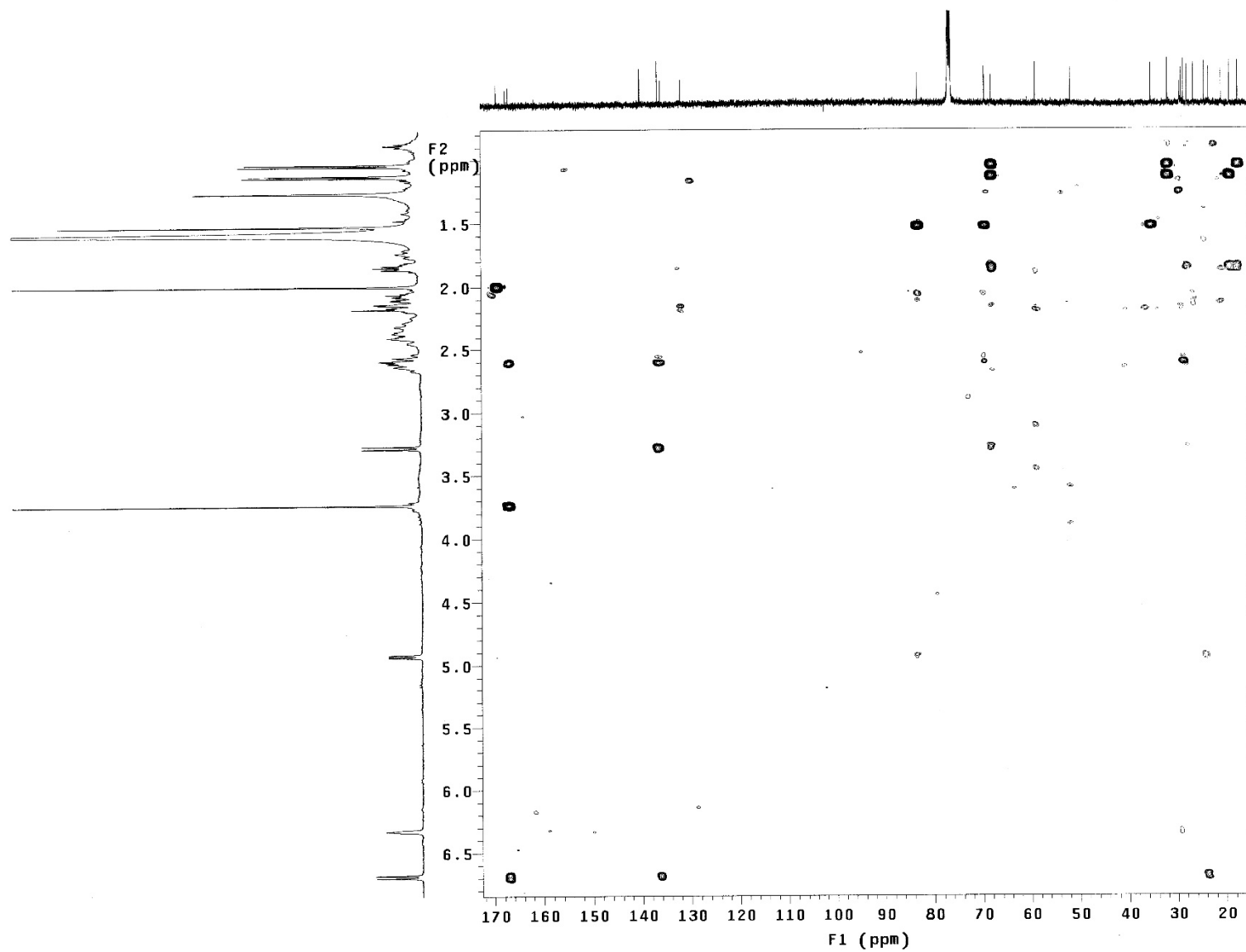


Figure S7. HMBC spectrum of **1** in CDCl_3 .

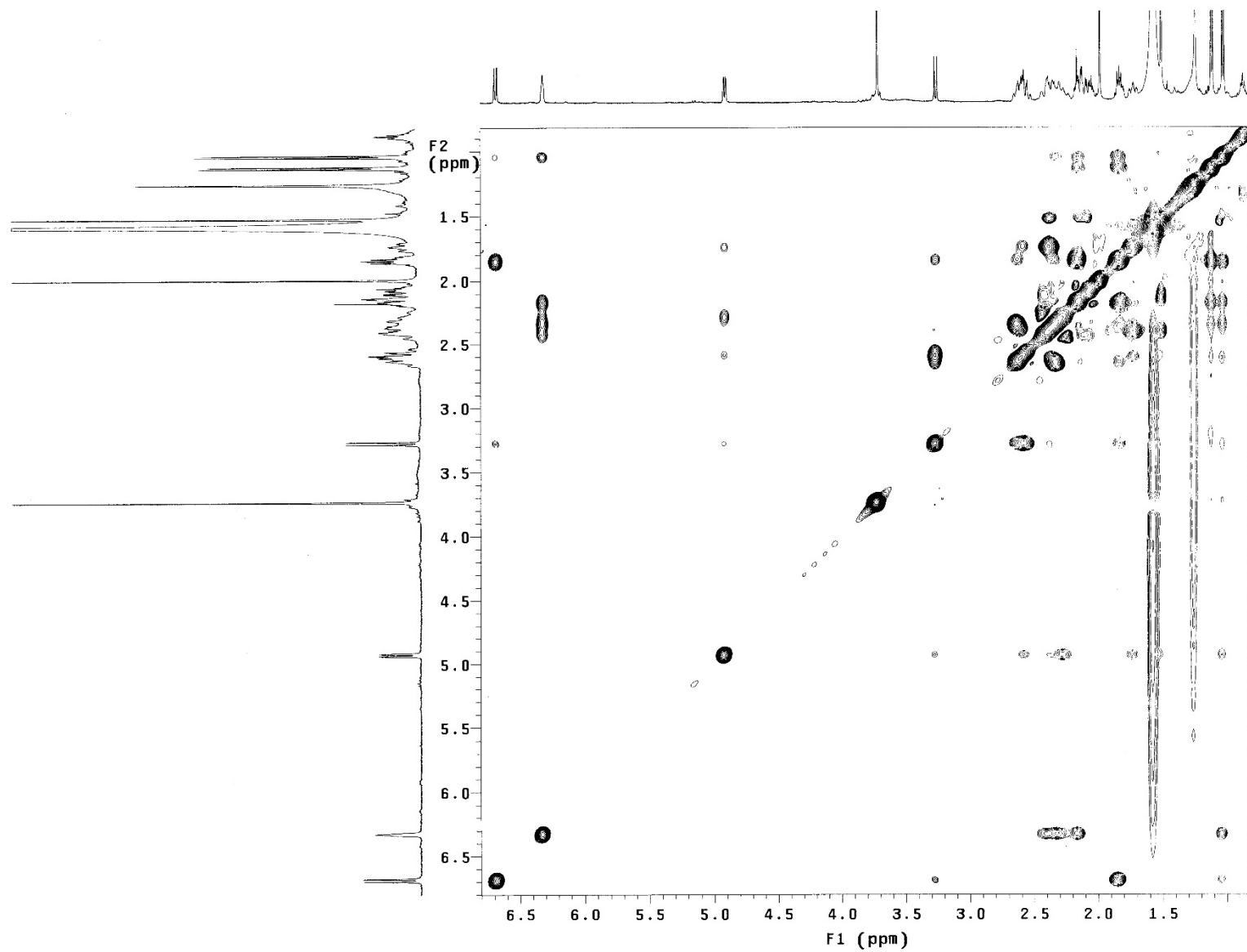
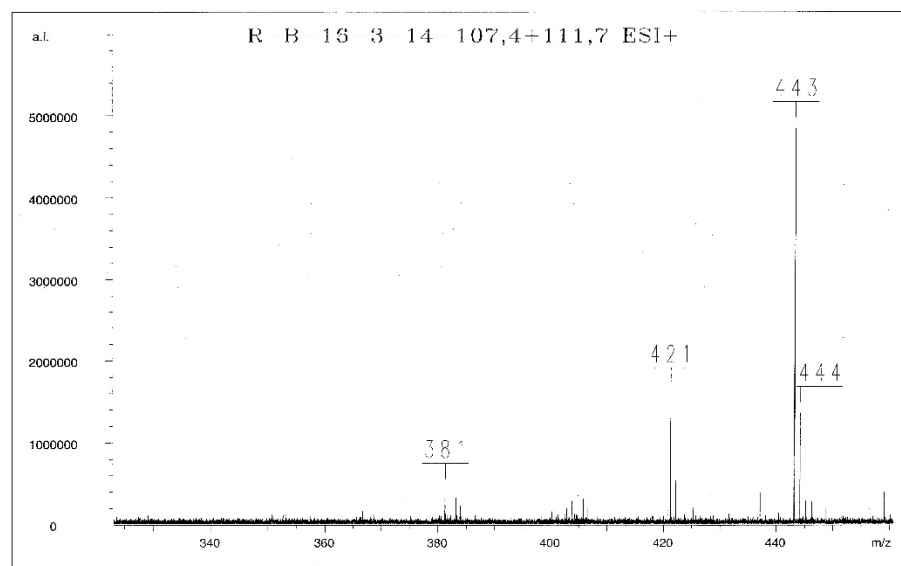
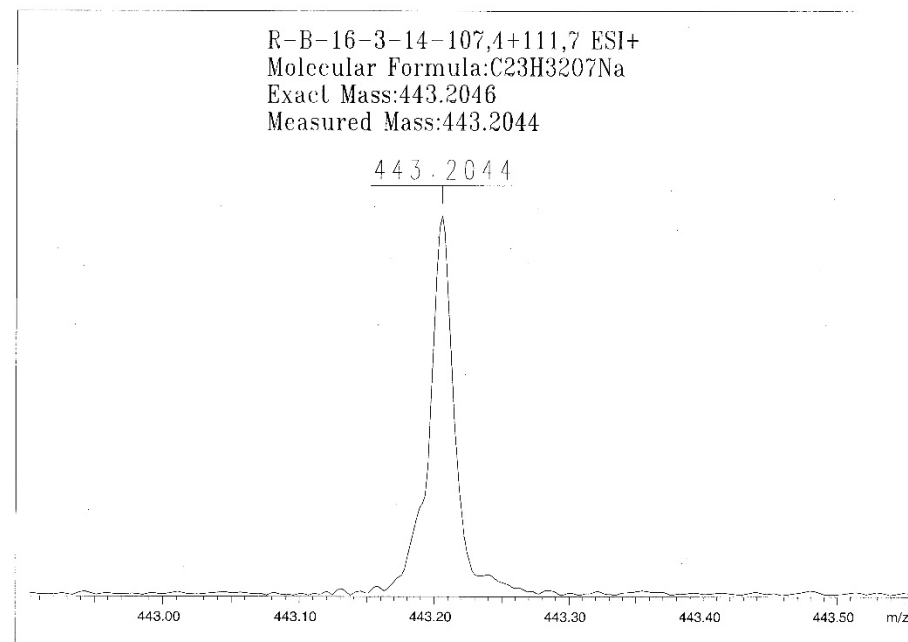


Figure S8. NOESY spectrum of **1** in CDCl_3 .



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Figure S9. LR- and HR-ESIMS spectra of **2**.

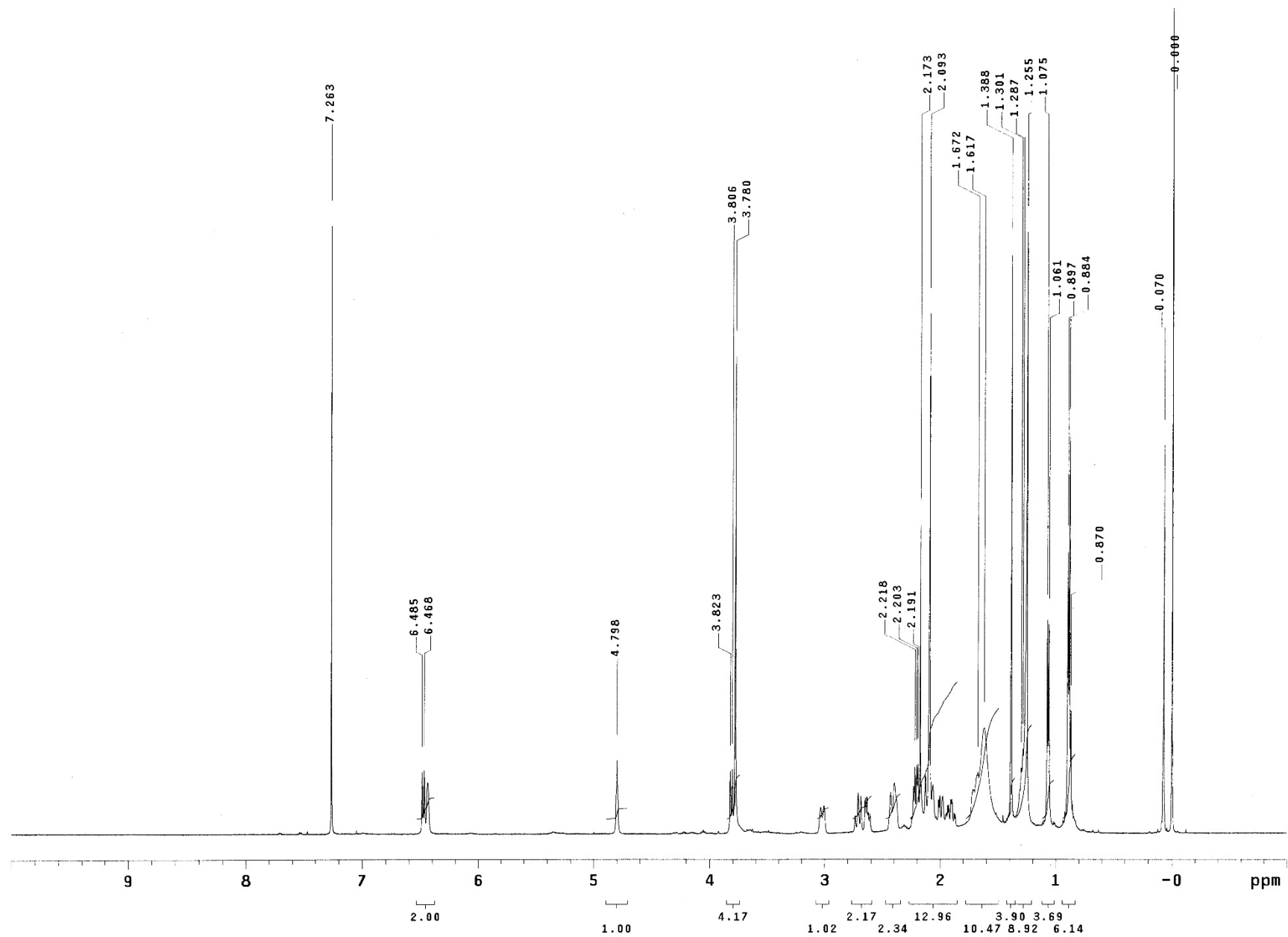


Figure S10. ¹H NMR spectrum of **2** in CDCl₃.

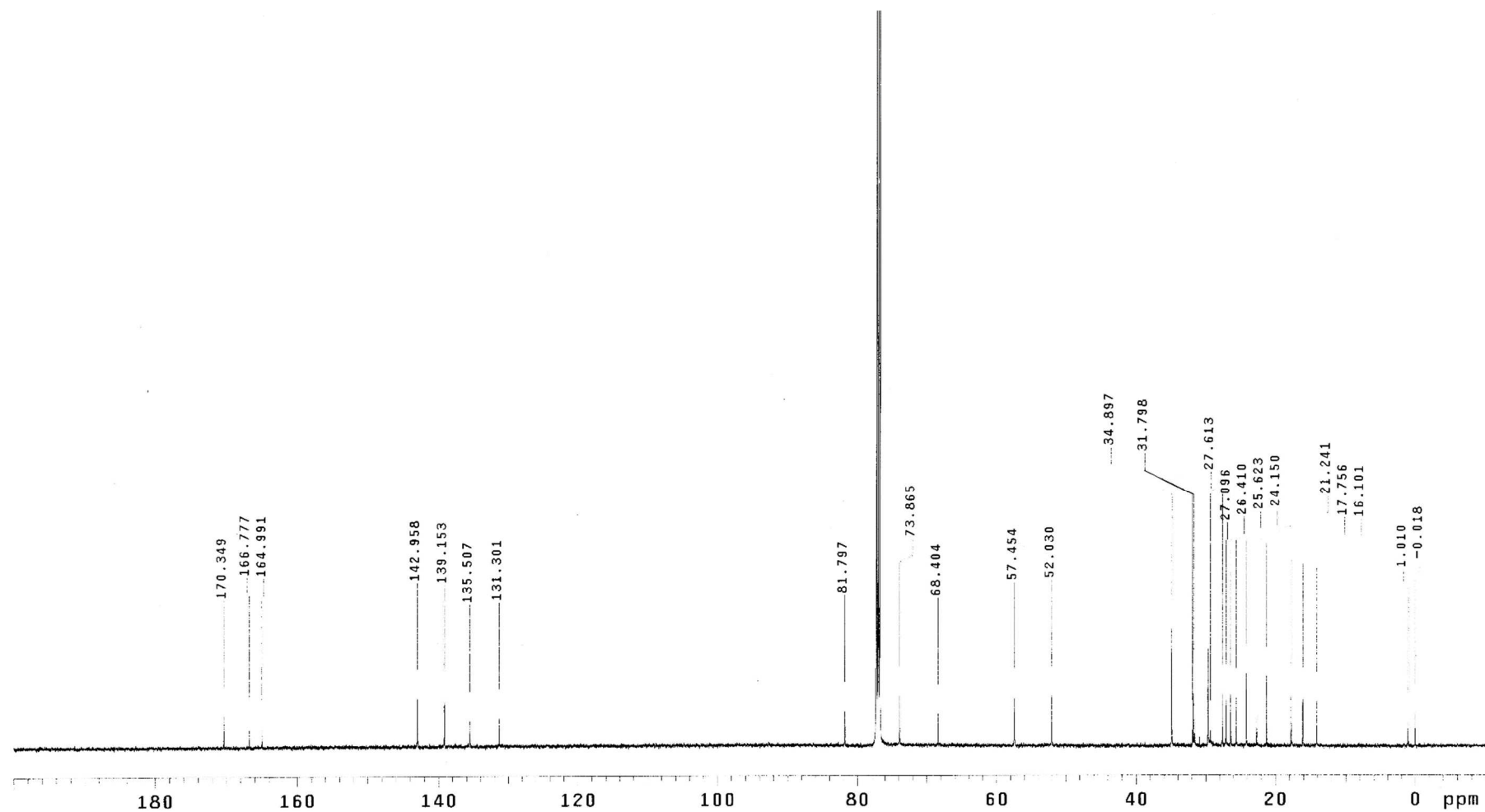


Figure S11. ¹³C NMR spectrum of **2** in CDCl₃.

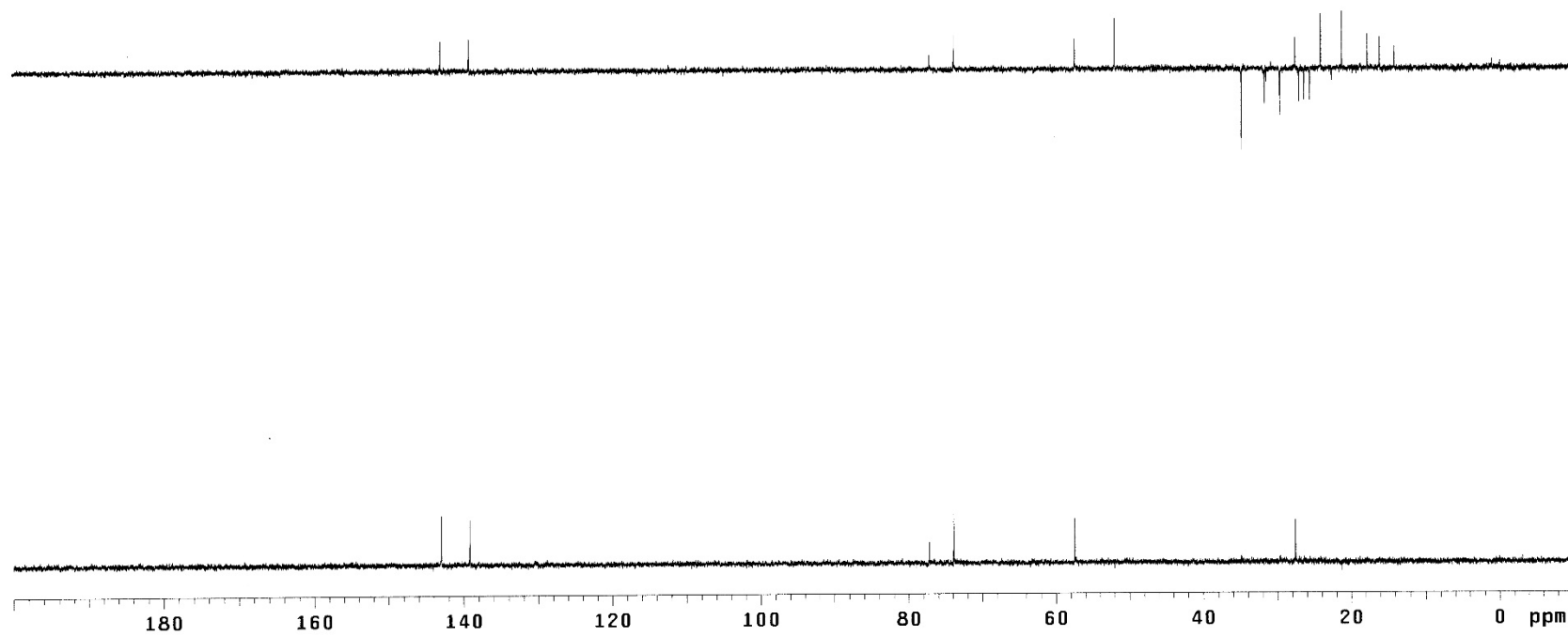


Figure S12. DEPT and ^{13}C NMR spectra of **2** in CDCl_3 .

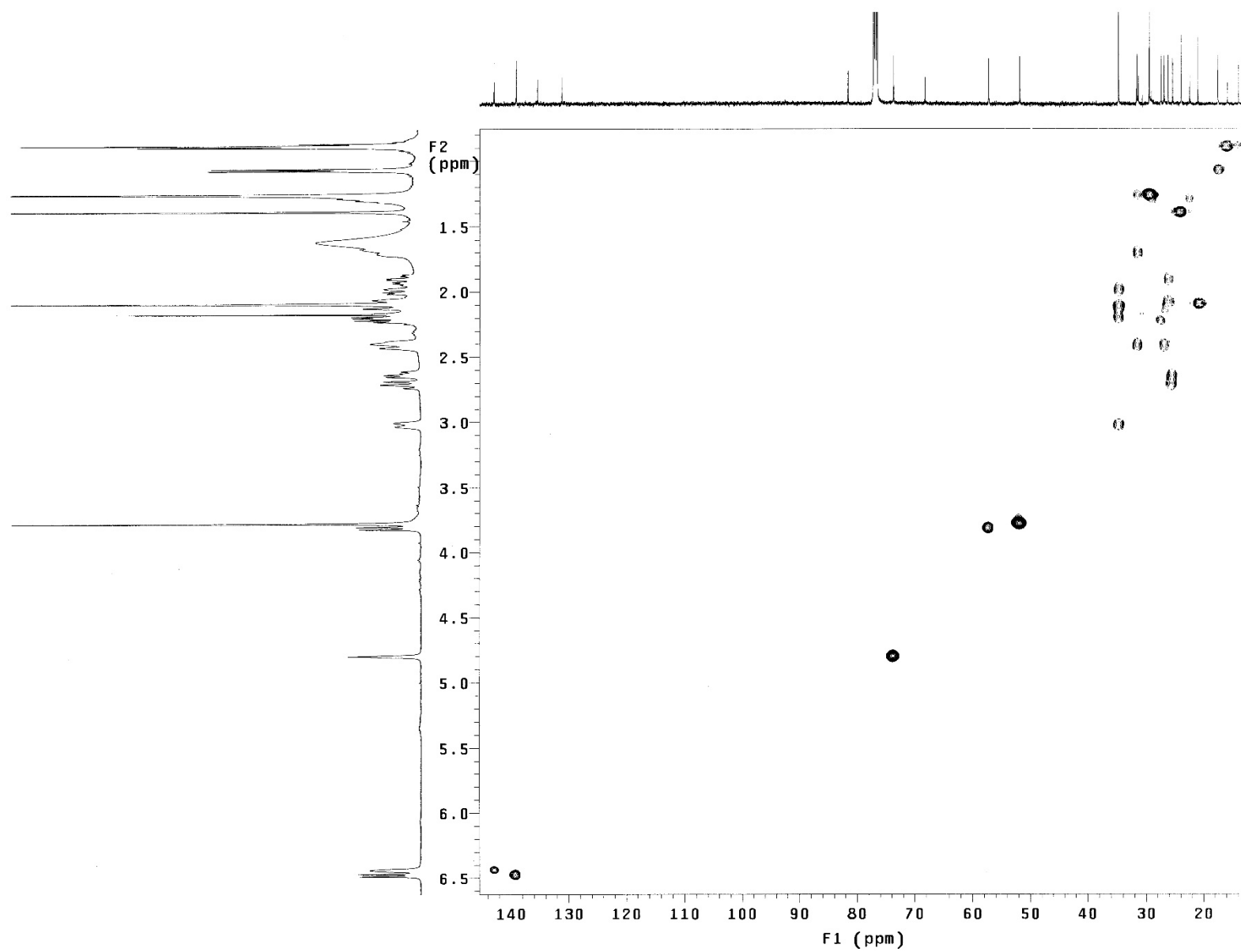


Figure S13. HSQC spectrum of **2** in CDCl₃.

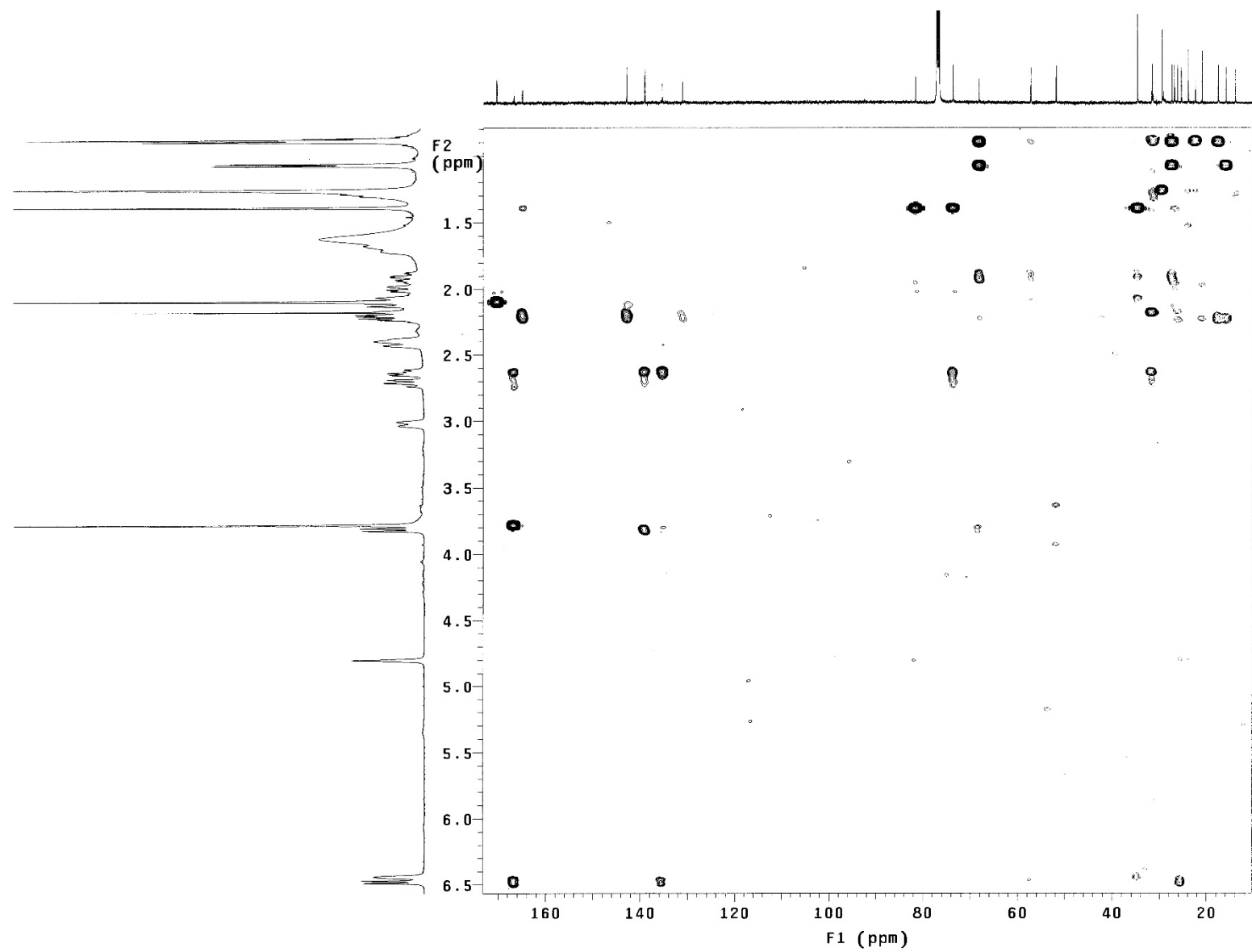


Figure S15. HMBC spectrum of **2** in CDCl_3 .

R-B-16-3-14-107.4-111.7

Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: vnmr1
File: NOESY
INNOVA-500 "NSYSU500"
Relax. delay 1.500 sec
Mixing 0.500 sec
Acq. time 0.292 sec
Width 3511.9 Hz
2D Width 3511.9 Hz
32 repetitions
2 x 128 increments
OBSERVE H1, 499.7179432 MHz
DATA PROCESSING
Gauss apodization 0.033 sec
F1 DATA PROCESSING
Gauss apodization 0.018 sec
FT size 2048 x 2048
Total time 5 hr, 23 min, 3 sec

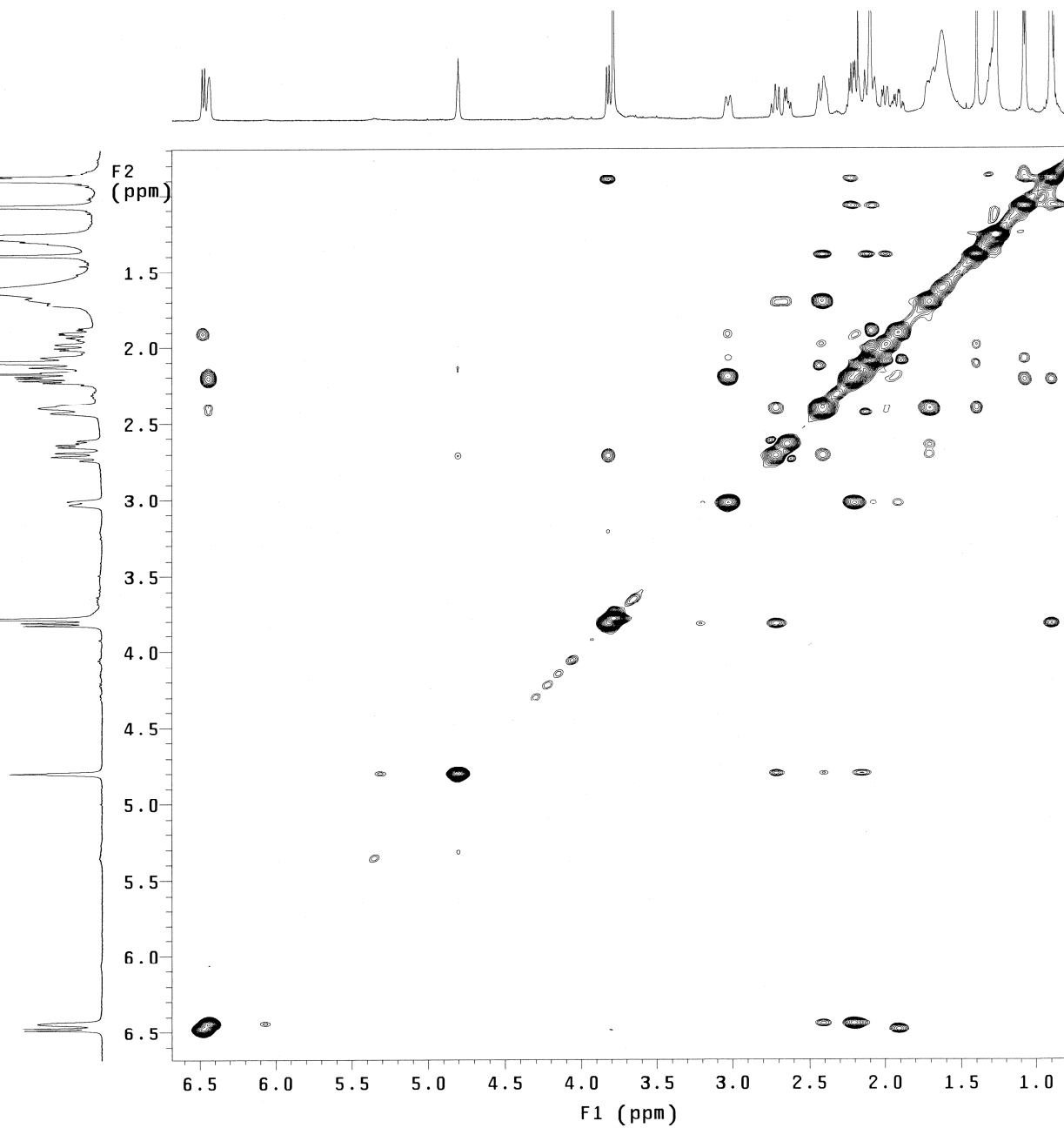
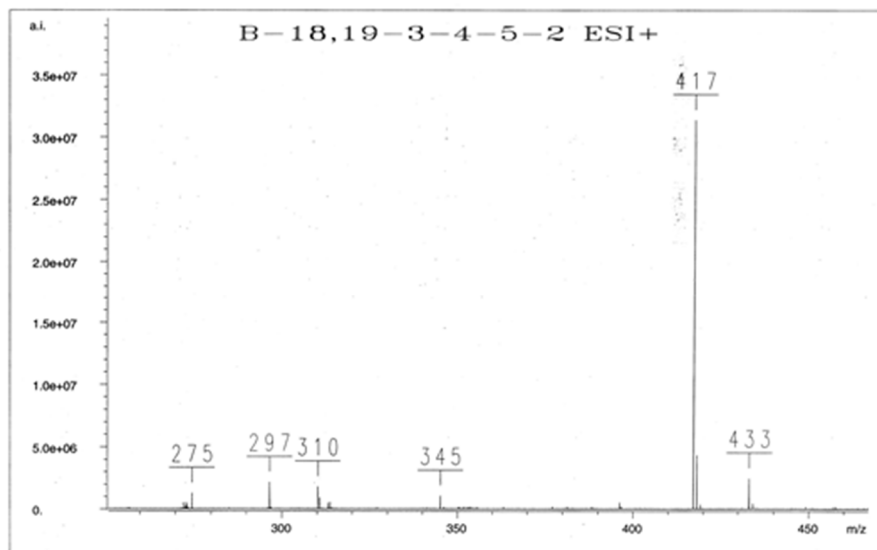
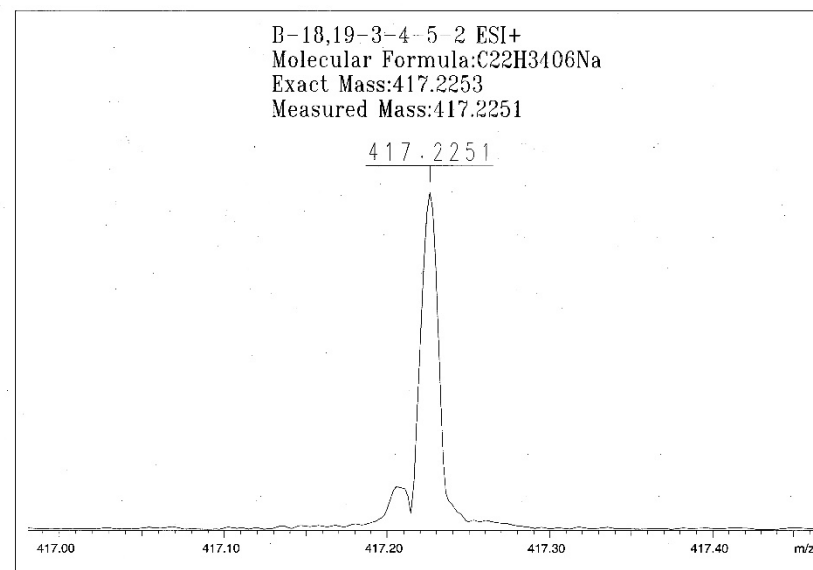


Figure S16. NOESY spectrum of **2** in CDCl₃.



/d=/Data/yu/b18193452/2/pdata/1 Administrator Mon Jul 30 16:03:20 2012



/d=/Data/yu/b18193452/3/pdata/1 Administrator Mon Jul 30 16:12:29 2012

Figure S17. LR- and HR-ESIMS spectra of **3**.

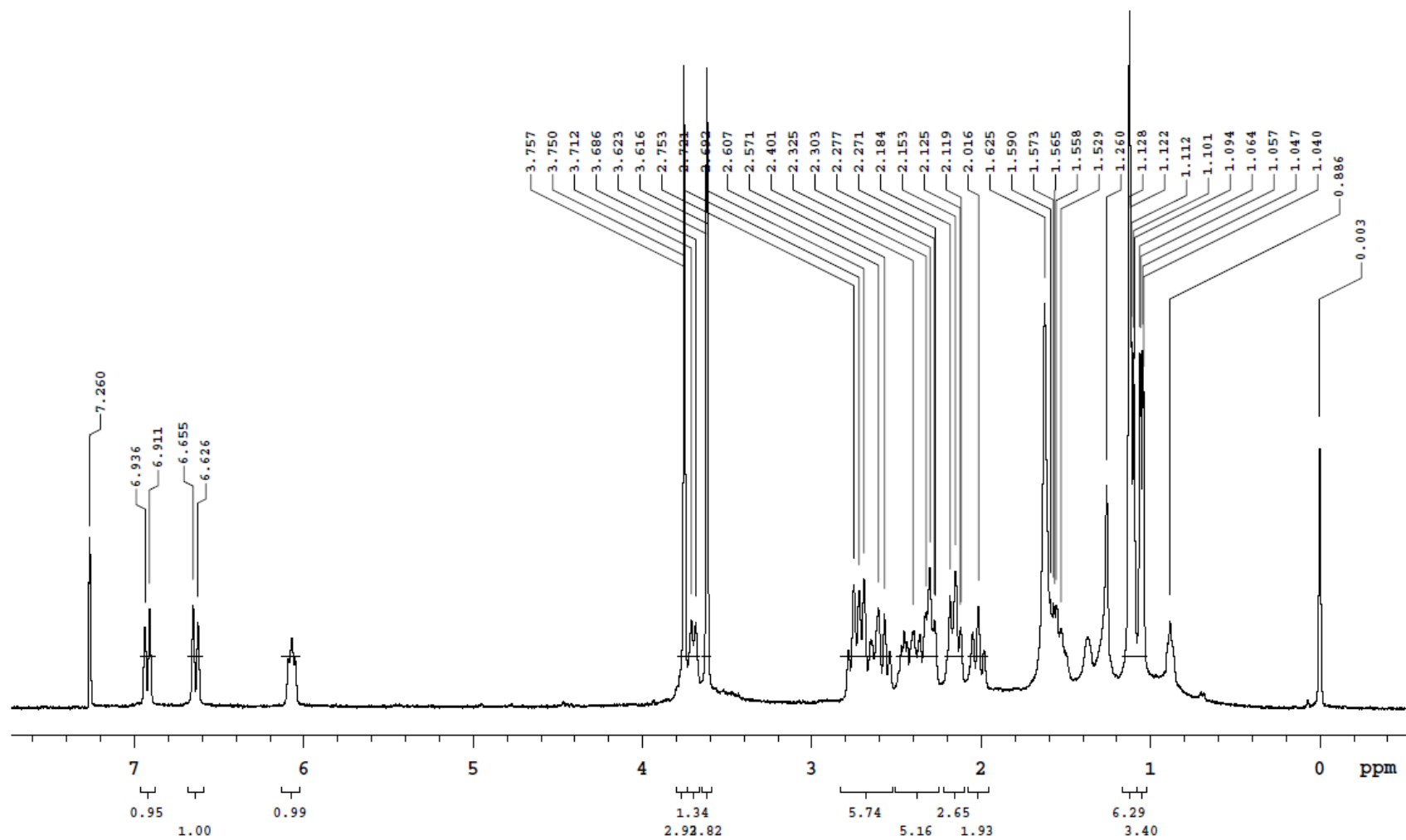


Figure S18. ¹H NMR spectrum of **3** in CDCl₃.

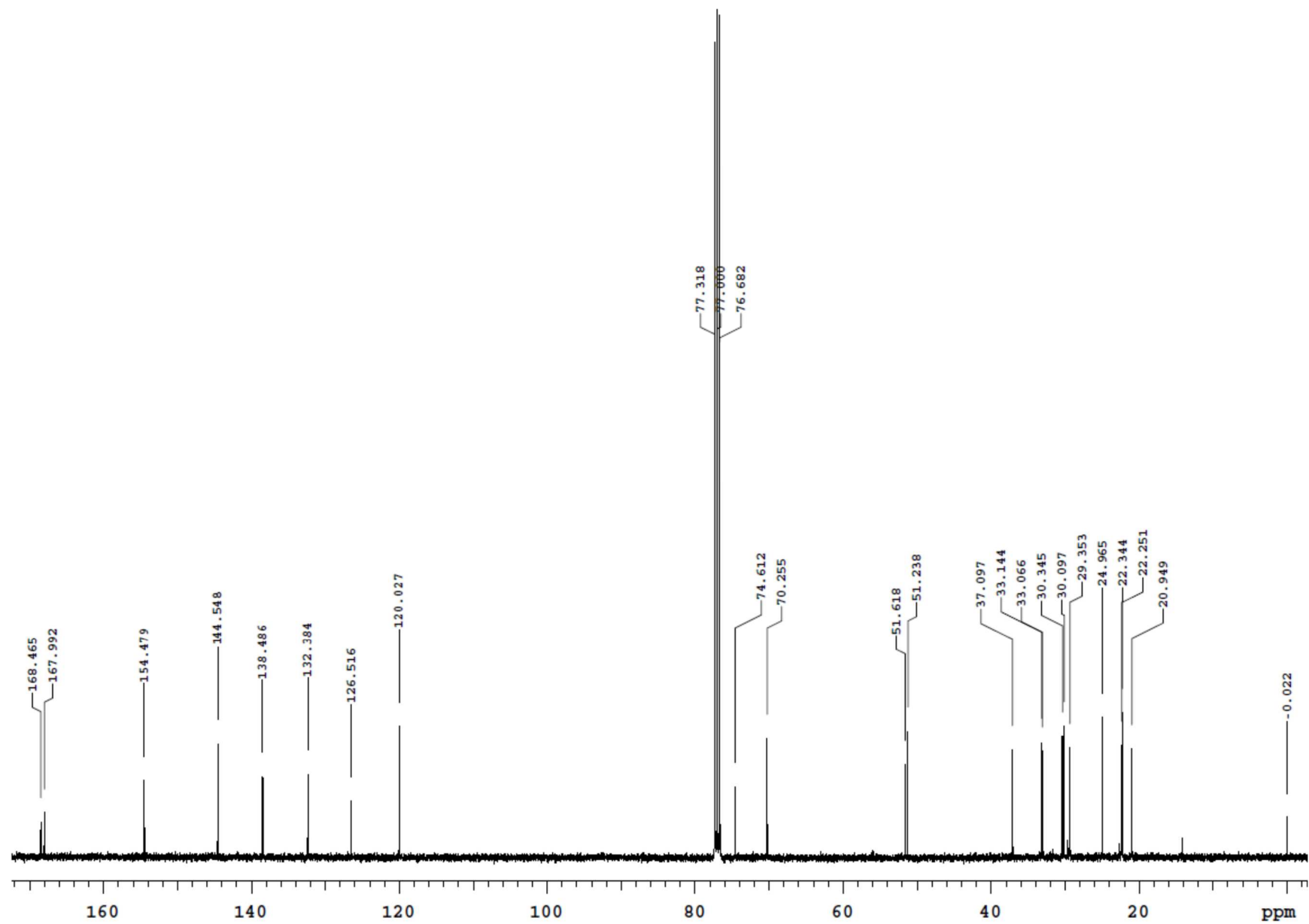


Figure S19. ¹³C NMR spectrum of **3** in CDCl₃.

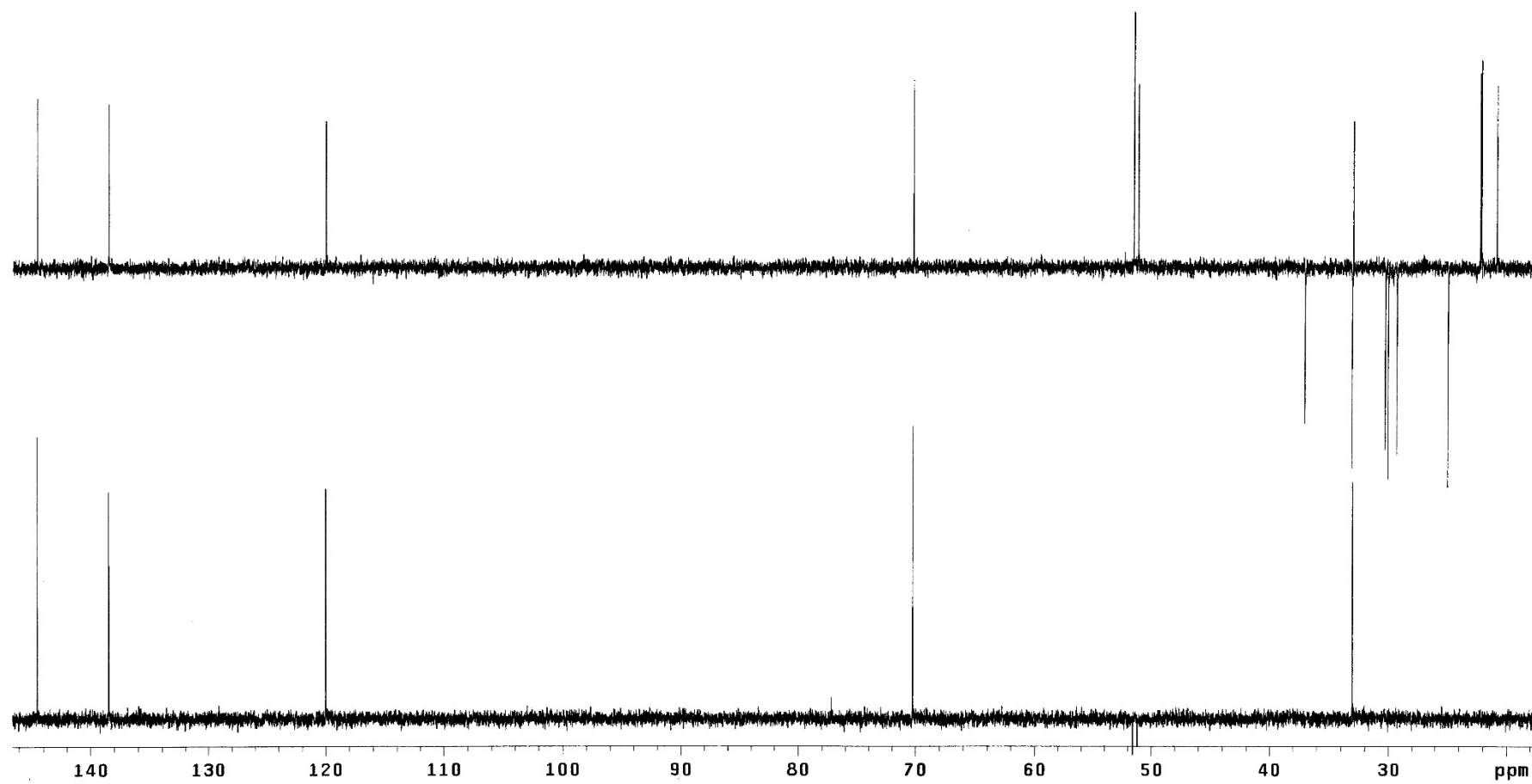


Figure S20. DEPT and ^{13}C NMR spectra of **3** in CDCl_3 .

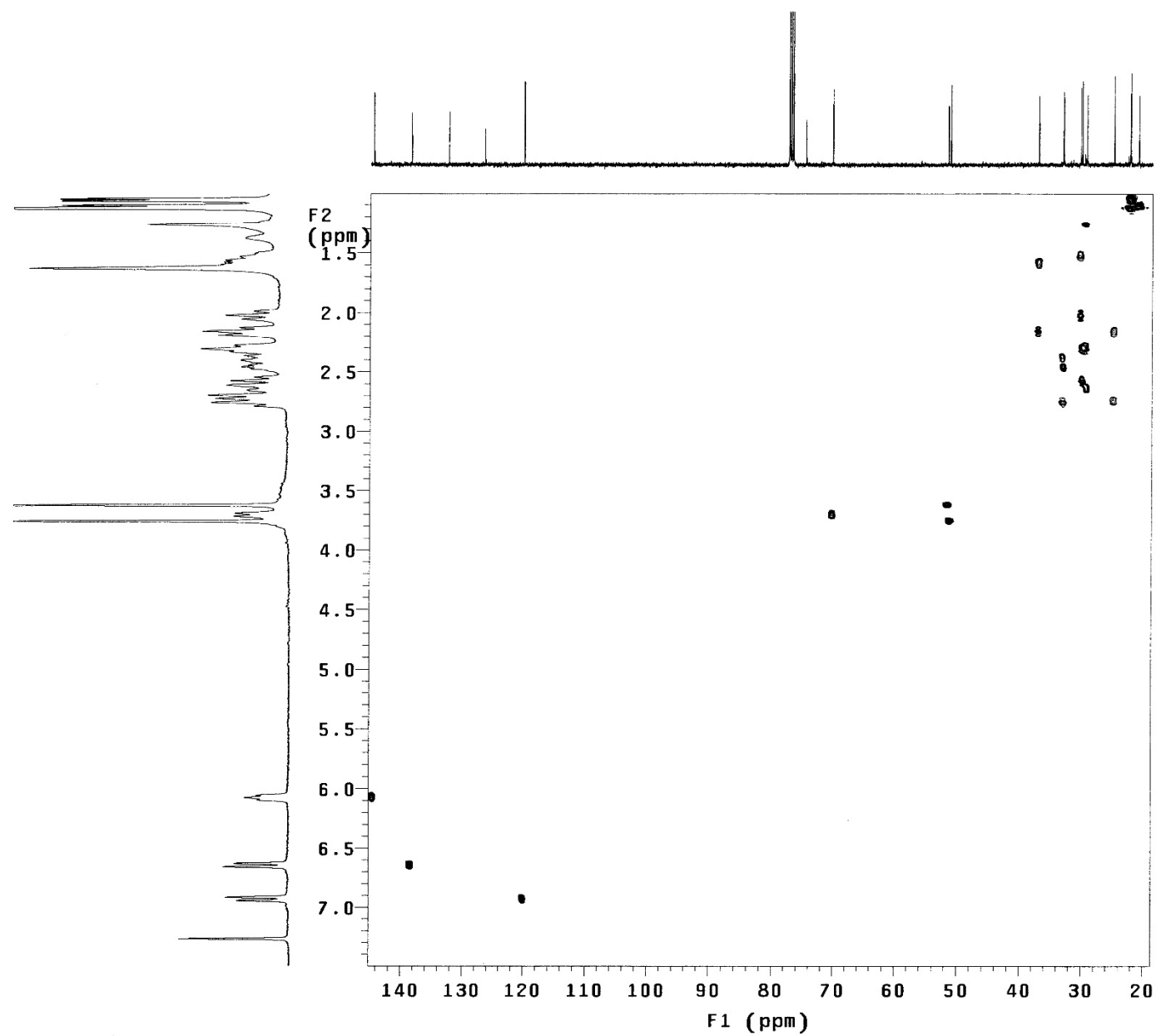


Figure S21. HSQC spectrum of **3** in CDCl₃.

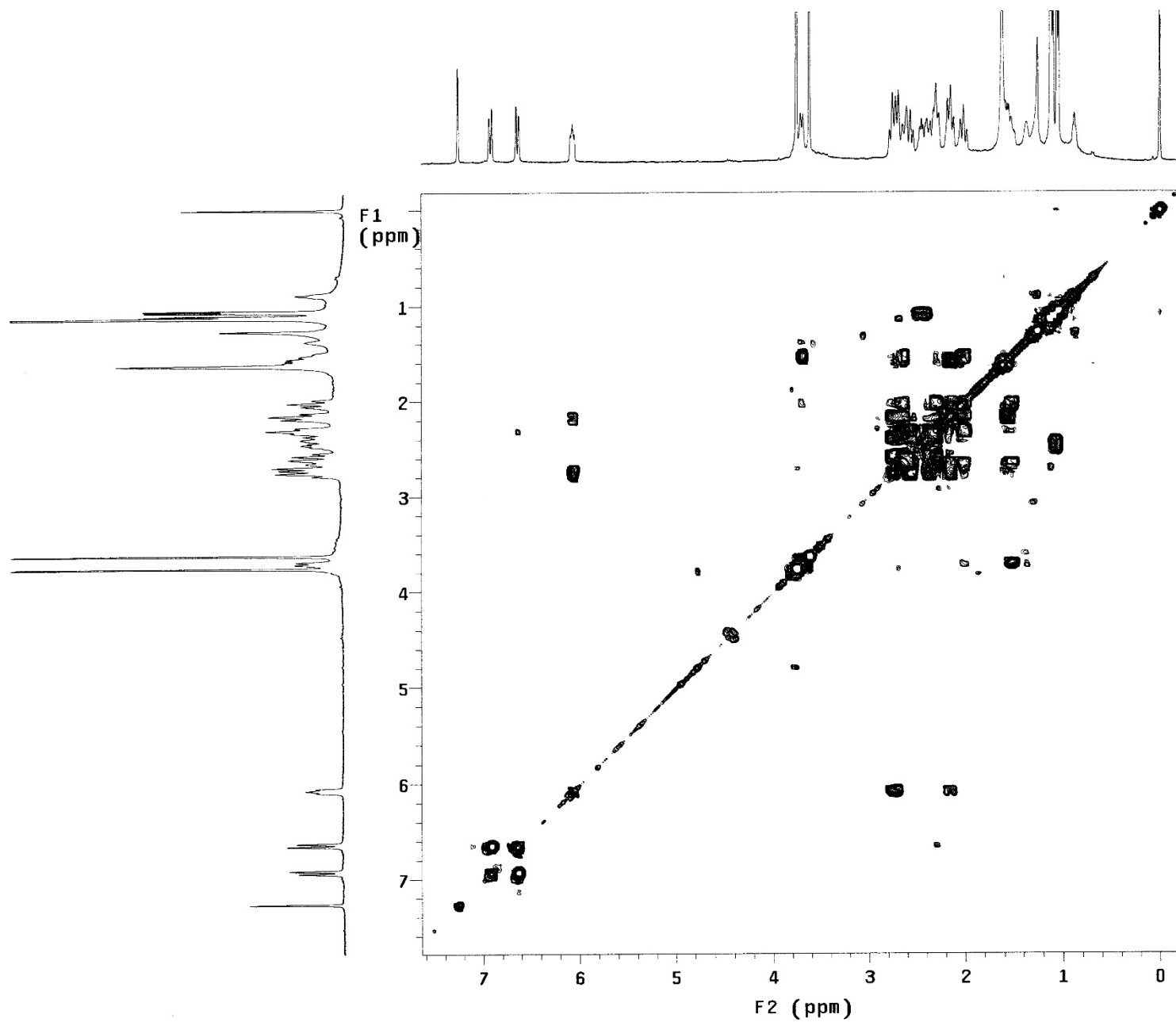


Figure S22. ^1H - ^1H COSY spectrum of **3** in CDCl_3 .

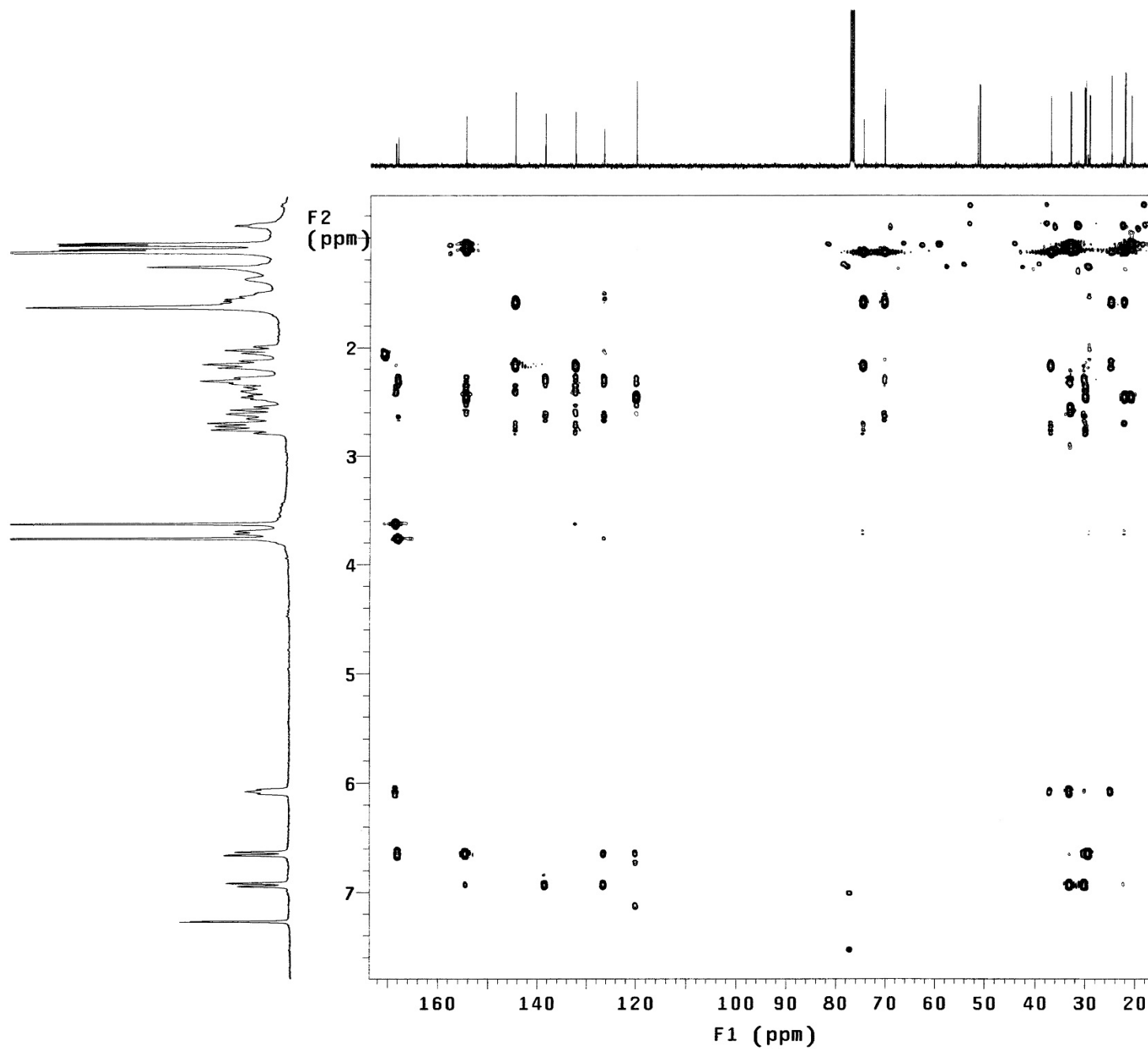


Figure S23. HMBC spectrum of **3** in CDCl₃.

exp12 NOESY

SAMPLE			FLAGS		
date	May 19 2012		hs		nn
solvent	cdcl3		sspul		y
sample	B-18_19-3-4~		pfgef1g		y
	-5-2_20120519_02		hsglv1		1020
ACQUISITION			SPECIAL		
sw	3742.5		temp	not	used
at	0.150		gain		30
np	1122		sp in	not	used
fb	4000		F2	PROCESSING	
ss	32		gf		0.069
d1	1.000		gfs	not	used
nt	44		fn		2048
2D ACQUISITION			F1 PROCESSING		
sw1	3742.5		gf1		0.049
ni	200		gfs1	not	used
TRANSMITTER					
tn	H1		proci		lp
sfrq	399.363		fn1		2048
tof	-553.3		DISPLAY		
tpwr	62		sp		-424.1
pw	8.250		wp		3738.9
			sp1		-424.1
			wp1		3738.9
mixN	0.500		rfl		427.7
PRESATURATION			rfp		0
satmode	n		rfl1		-427.7
wet	n		rfp1		0
DECOUPLER			PLOT		
dn	C13		wc		130.0
dm	nnn		sc		6.7
			wc2		130.0
			sc2		0
			vs		1471
			th		1
			ai	ph	

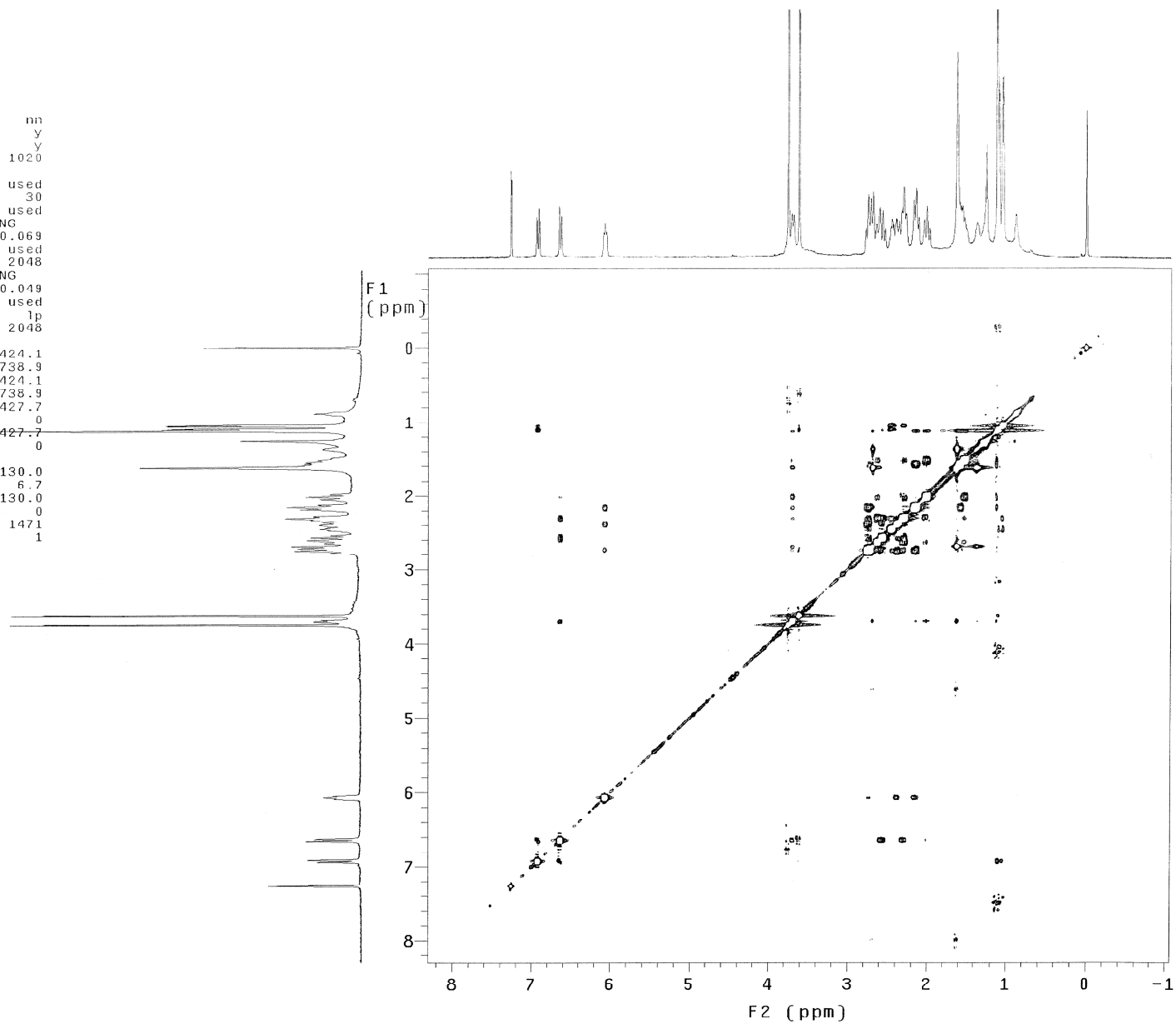


Figure S24. NOESY spectrum of **3** in CDCl₃.

Table S1. Low-energy conformers of 1*R*,2*S*,7*S*,8*R*-1 for ECD calculations.

Conformer 1a (97.39%)				Conformer 1b (1.23%)			
C	2.904927	1.06325	0.256427	C	-2.41811	-1.72247	0.46399
C	2.878808	1.897627	-1.02391	C	-2.34163	-2.64425	-0.75443
C	4.284187	2.072305	-1.59999	C	-3.72198	-3.1858	-1.128
C	1.90126	1.388301	-2.08335	C	-1.62883	-2.04076	-1.96645
C	1.774619	1.145708	1.220206	C	-1.1983	-1.48513	1.289021
C	3.756667	-0.18802	0.332708	C	-3.53517	-0.70133	0.562309
O	2.990907	1.849364	1.435386	O	-2.20049	-2.41143	1.685449
C	0.572082	1.952948	0.943683	C	0.11259	-2.02721	0.883689
C	-0.67765	1.661168	1.33869	C	1.326235	-1.52047	1.157058
C	3.342914	-1.35379	-0.57191	C	-3.57955	0.379838	-0.52493
C	1.896328	-1.81916	-0.50627	C	-2.36223	1.282142	-0.6081
C	1.466101	-2.23491	0.873343	C	-2.17545	2.111395	0.629818
O	0.187197	-2.3821	1.26265	O	-1.05651	2.791542	0.918345
C	-1.02176	-2.54716	0.496306	C	0.211939	2.811558	0.240404
C	-0.78032	-3.29252	-0.8143	C	0.038231	3.223194	-1.22018
C	-0.14478	-2.49712	-1.93476	C	-0.46711	2.147748	-2.16348
C	1.206869	-1.94078	-1.65438	C	-1.6762	1.372668	-1.7621
O	2.303041	-2.38444	1.731948	O	-3.07601	2.195464	1.431042
C	-1.60665	-1.1368	0.270995	C	0.876596	1.42441	0.411568
C	-2.1181	-0.41621	1.521734	C	0.958879	0.98154	1.864133
C	-1.09638	0.499882	2.202889	C	1.662871	-0.3658	2.079072
C	-1.79087	2.580011	0.943422	C	2.449849	-2.23345	0.455508
O	-2.68988	-1.31573	-0.64964	O	2.203151	1.533058	-0.11407
C	-1.91347	-3.41583	1.378323	C	0.990643	3.901122	0.97074
C	-3.06848	-0.23955	-1.35711	C	2.638528	0.682797	-1.05792
C	-4.21773	-0.55613	-2.2673	C	4.073723	0.956701	-1.39651
O	-2.52653	0.831746	-1.25142	O	1.950648	-0.16992	-1.55921
O	-2.87878	2.572818	1.469319	O	2.336496	-3.26786	-0.15498
O	-1.47234	3.416162	-0.04313	O	3.618415	-1.59036	0.548474
C	-2.52195	4.249884	-0.51395	C	4.707305	-2.18329	-0.14942
H	2.537366	2.892275	-0.7023	H	-1.74847	-3.50343	-0.41083
H	4.268014	2.79918	-2.42434	H	-4.37245	-2.39233	-1.52661
H	4.674311	1.123892	-2.00038	H	-3.6264	-3.95808	-1.90436
H	4.985983	2.43731	-0.83561	H	-4.22196	-3.63593	-0.25772
H	2.263247	0.463641	-2.55199	H	-2.27996	-1.34355	-2.51044

H	1.794609	2.138284	-2.88046	H	-1.35573	-2.84044	-2.67013
H	0.902427	1.193751	-1.66171	H	-0.70804	-1.50614	-1.68291
H	1.649038	0.28688	1.888275	H	-1.19081	-0.57711	1.899174
H	3.748578	-0.51719	1.379303	H	-3.4666	-0.22506	1.55002
H	4.797939	0.079423	0.094844	H	-4.49248	-1.24573	0.547358
H	0.722292	2.856725	0.351215	H	0.093462	-2.91272	0.245811
H	3.568282	-1.11386	-1.62073	H	-3.74104	-0.07927	-1.50987
H	3.984448	-2.20843	-0.30585	H	-4.45904	1.007501	-0.31942
H	-0.15819	-4.17104	-0.57746	H	1.006781	3.589919	-1.58961
H	-1.75159	-3.67407	-1.15591	H	-0.645	4.086898	-1.22041
H	-0.05522	-3.14125	-2.82356	H	0.321586	1.399865	-2.35893
H	-0.80004	-1.67067	-2.26081	H	-0.66921	2.598203	-3.14792
H	1.734989	-1.60918	-2.55366	H	-2.05283	0.740348	-2.57149
H	-0.83553	-0.51773	-0.21898	H	0.326894	0.67241	-0.17366
H	-2.501	-1.14027	2.251404	H	1.516788	1.734481	2.43844
H	-2.97564	0.198707	1.221772	H	-0.05766	0.981089	2.277567
H	-0.22431	-0.0821	2.525406	H	1.464146	-0.68599	3.114079
H	-1.57011	0.908189	3.108664	H	2.743071	-0.19632	2.019705
H	-2.94879	-3.37738	1.012577	H	0.931712	3.761547	2.056907
H	-1.5632	-4.45621	1.34311	H	2.041721	3.885536	0.657457
H	-1.88324	-3.08088	2.42143	H	0.55892	4.88128	0.727272
H	-4.49369	0.336278	-2.83598	H	4.680757	0.863864	-0.48632
H	-3.93187	-1.36973	-2.94701	H	4.415317	0.252852	-2.16097
H	-5.06871	-0.90574	-1.6681	H	4.171011	1.988538	-1.75991
H	-3.33678	3.630097	-0.91089	H	5.574702	-1.54044	0.026565
H	-2.09223	4.867994	-1.30746	H	4.897986	-3.19578	0.228555
H	-2.91012	4.881822	0.295249	H	4.480351	-2.24087	-1.22263
Conformer 1c (1.11%)							
C	2.454268	1.69774	0.284003				
C	2.299563	2.850115	-0.70267				
C	3.63225	3.573899	-0.90309				
C	1.682769	2.409101	-2.0288				
C	1.302771	1.294628	1.139667				
C	3.583505	0.71435	-0.00823				
O	2.354501	2.111429	1.637173				
C	-0.0467	1.868548	0.952755				
C	-1.1941	1.305514	1.370296				

C	3.380681	-0.71485	0.479423
C	2.255647	-1.49041	-0.18999
C	1.894046	-2.71885	0.59055
O	0.68348	-3.28729	0.533962
C	-0.46547	-2.86396	-0.22636
C	-0.12112	-2.89674	-1.7174
C	0.667941	-1.70329	-2.23776
C	1.765105	-1.14261	-1.39097
O	2.702641	-3.21484	1.336877
C	-0.95158	-1.46909	0.262309
C	-0.79375	-1.25619	1.758817
C	-1.3571	0.086679	2.256914
C	-2.4818	1.920744	0.904711
O	-2.33885	-1.35814	-0.07356
C	-1.49335	-3.94642	0.087741
C	-2.73992	-0.49124	-1.01771
C	-4.21954	-0.58802	-1.24131
O	-1.99515	0.265841	-1.58864
O	-3.56854	1.427474	1.102263
O	-2.32824	3.049368	0.21737
C	-3.50953	3.606807	-0.34582
H	1.61887	3.5679	-0.22369
H	4.068613	3.865581	0.063476
H	4.359788	2.942508	-1.43453
H	3.483333	4.484487	-1.50039
H	1.462719	3.285656	-2.65454
H	0.743097	1.854778	-1.8741
H	2.373471	1.769817	-2.60083
H	1.321026	0.285476	1.554427
H	4.488411	1.121372	0.468902
H	3.794186	0.722141	-1.08752
H	-0.12188	2.786145	0.36979
H	3.206537	-0.71212	1.566857
H	4.3182	-1.27787	0.352697
H	-1.05493	-2.97477	-2.29382
H	0.426309	-3.83675	-1.88658
H	-0.02071	-0.86245	-2.42893
H	1.091552	-1.94584	-3.22584

H	2.216596	-0.25825	-1.84681
H	-0.41799	-0.66989	-0.26347
H	-1.29491	-2.06736	2.307432
H	0.271807	-1.34314	2.008961
H	-0.90284	0.302826	3.235572
H	-2.43248	-0.03194	2.429919
H	-1.70506	-3.98045	1.164788
H	-2.42738	-3.76327	-0.45373
H	-1.08328	-4.91865	-0.21623
H	-4.50512	-1.63392	-1.41076
H	-4.72325	-0.23237	-0.33279
H	-4.50291	0.034177	-2.09552
H	-3.95596	2.899503	-1.05783
H	-3.20157	4.520996	-0.8607
H	-4.24066	3.836028	0.439632

Table S2. Low-energy conformers of **2** for ECD calculations.

Conformer 2a (48.13%)				Conformer 2b (45.14%)			
C	-2.28069	-1.67214	-0.34339	C	-2.69265	-0.9427	-0.3581
C	-3.50098	-0.77628	-0.5642	C	-3.6151	0.275237	-0.29273
C	-3.52106	-0.11075	-1.93876	C	-3.52398	1.173237	-1.52486
C	-4.77166	-1.60368	-0.34501	C	-5.05543	-0.19659	-0.07104
C	-1.09421	-1.56332	-1.24302	C	-1.60786	-1.00538	-1.3806
C	-2.11826	-2.26256	1.047537	C	-2.58777	-1.77432	0.908205
O	-2.06374	-2.59349	-1.3952	O	-2.82877	-1.716	-1.53648
C	0.242271	-2.04354	-0.84235	C	-0.39485	-1.81895	-1.17441
C	1.42418	-1.47965	-1.13551	C	0.855001	-1.46604	-1.5167
C	-2.16524	-1.23534	2.185468	C	-2.18399	-0.98688	2.158597
C	-1.24086	-0.04084	2.023594	C	-0.94891	-0.11376	2.02014
C	0.216485	-0.40504	2.141334	C	0.312723	-0.90869	1.804493
O	1.241927	0.430752	1.89362	O	1.48312	-0.39464	1.385763
C	1.238366	1.756047	1.332368	C	1.877043	0.974256	1.171383
C	0.262742	2.683096	2.054956	C	1.380361	1.889049	2.291173
C	-1.20496	2.532813	1.720783	C	-0.07401	2.307415	2.242232
C	-1.79472	1.177282	1.883233	C	-1.0792	1.212	2.205117
O	0.511438	-1.51916	2.502836	O	0.288872	-2.10205	1.988874
C	0.932545	1.583911	-0.17084	C	1.353491	1.390109	-0.2233
C	2.072335	0.940592	-0.97273	C	2.083486	0.767164	-1.42427
C	1.644016	-0.20373	-1.90182	C	1.25181	-0.21484	-2.25167
C	2.626924	-2.21265	-0.61585	C	1.988206	-2.36284	-1.13101
O	0.657193	2.895537	-0.67836	O	1.482379	2.816971	-0.27833
C	2.646857	2.287306	1.583876	C	3.401313	0.935497	1.237187
C	-0.1726	2.998146	-1.72653	C	0.700995	3.451941	-1.16541
C	-0.37898	4.429504	-2.12475	C	0.907619	4.937057	-1.11984
O	-0.68444	2.041492	-2.25165	O	-0.07063	2.868838	-1.8842
O	2.598504	-3.22835	0.034733	O	3.150951	-2.08857	-1.32303
O	3.770123	-1.61721	-0.96569	O	1.607852	-3.49627	-0.54601
C	4.966852	-2.24064	-0.51486	C	2.647059	-4.33337	-0.05936
H	-3.46689	0.017118	0.196021	H	-3.30254	0.867445	0.581011
H	-2.71242	0.623937	-2.05356	H	-2.54806	1.673335	-1.59968
H	-4.47611	0.412537	-2.08542	H	-4.29727	1.952295	-1.47792
H	-3.42386	-0.86907	-2.73071	H	-3.69003	0.58519	-2.44067
H	-4.78722	-2.45975	-1.03724	H	-5.36173	-0.8637	-0.89154

H	-5.66434	-0.99224	-0.53677	H	-5.74178	0.661289	-0.05207
H	-4.846	-1.9906	0.681159	H	-5.17432	-0.74055	0.876514
H	-1.12224	-0.78859	-2.01466	H	-1.50684	-0.14574	-2.0464
H	-1.17888	-2.82217	1.104499	H	-1.88404	-2.59808	0.751509
H	-2.92469	-2.99563	1.204314	H	-3.56791	-2.24156	1.090163
H	0.269112	-2.97856	-0.27921	H	-0.53262	-2.77798	-0.67594
H	-3.19055	-0.85595	2.298817	H	-3.01659	-0.34479	2.478544
H	-1.91236	-1.75729	3.119048	H	-2.01147	-1.71011	2.968638
H	0.567522	3.716222	1.8401	H	2.005945	2.791528	2.281214
H	0.419916	2.522418	3.133335	H	1.589366	1.367396	3.239082
H	-1.78659	3.226436	2.347594	H	-0.29616	2.925769	3.126562
H	-1.41275	2.860174	0.687404	H	-0.26639	2.975933	1.386967
H	-2.88985	1.187124	1.880987	H	-2.10254	1.55739	2.388702
H	0.012201	0.98194	-0.26292	H	0.278193	1.143468	-0.26848
H	2.556579	1.740425	-1.55205	H	2.389654	1.591724	-2.08313
H	2.837633	0.549051	-0.29244	H	3.005577	0.269274	-1.10989
H	2.443874	-0.37356	-2.63509	H	1.857272	-0.51258	-3.12149
H	0.738157	0.081241	-2.45058	H	0.364354	0.306478	-2.63178
H	2.755335	2.556462	2.643133	H	3.722713	0.859017	2.28464
H	3.409749	1.539556	1.342202	H	3.79388	0.067724	0.694562
H	2.813947	3.185339	0.973252	H	3.816741	1.856832	0.805585
H	-1.02543	4.477157	-3.00545	H	0.319254	5.414663	-1.90832
H	-0.83592	4.975299	-1.28803	H	0.595486	5.314499	-0.13628
H	0.592632	4.895046	-2.33413	H	1.974166	5.165017	-1.24077
H	5.041206	-3.25928	-0.91683	H	2.15812	-5.21213	0.37055
H	4.981981	-2.28854	0.581681	H	3.227353	-3.80719	0.710527
H	5.79206	-1.62414	-0.88204	H	3.319723	-4.62974	-0.87444
Conformer 2c (1.64%)				Conformer 2d (1.59%)			
C	3.049806	-0.22021	-0.52958	C	0.269877	2.470082	-0.67802
C	3.451032	-1.66357	-0.82564	C	1.780452	2.706742	-0.72853
C	4.814548	-1.99527	-0.22092	C	2.442519	2.117326	-1.97055
C	2.393707	-2.69873	-0.4434	C	2.048103	4.214589	-0.6551
C	2.146449	0.42364	-1.52178	C	-0.37989	1.421017	-1.53236
C	3.176236	0.335643	0.877254	C	-0.43745	2.981751	0.569074
O	3.541528	0.686102	-1.50649	O	-0.39532	2.798641	-1.88298
C	1.277861	1.564002	-1.17076	C	-1.70471	0.874436	-1.17249
C	-0.01906	1.703655	-1.48861	C	-2.12216	-0.39968	-1.23404

C	2.392344	-0.34486	2.003062	C	0.235403	2.653635	1.90742
C	0.881704	-0.44901	1.871026	C	0.638123	1.215483	2.146439
C	0.19583	0.88083	1.712074	C	-0.43451	0.189587	2.001753
O	-1.04402	1.038937	1.213048	O	-0.12683	-1.12555	2.077984
C	-2.08178	0.061361	1.003354	C	0.926879	-1.84588	1.403479
C	-2.15359	-0.91409	2.180754	C	2.341992	-1.31343	1.701558
C	-1.13172	-2.03308	2.198043	C	2.375658	-0.45562	2.96457
C	0.299924	-1.63846	2.102667	C	1.843158	0.9135	2.660451
O	0.792386	1.887604	2.008352	O	-1.59861	0.498691	1.940006
C	-1.82999	-0.6615	-0.34364	C	0.636928	-1.75668	-0.10534
C	-2.07193	0.147751	-1.62568	C	-0.6999	-2.35237	-0.53773
C	-0.82773	0.731045	-2.3032	C	-1.3485	-1.59873	-1.71202
C	-0.753	2.913825	-1.01014	C	-3.46396	-0.73447	-0.66285
O	-2.74109	-1.77051	-0.33281	O	1.720634	-2.4598	-0.72807
C	-3.36477	0.885585	0.982042	C	0.785488	-3.26801	1.927712
C	-2.41242	-2.8344	-1.08223	C	2.201945	-2.04631	-1.90551
C	-3.44693	-3.9166	-0.98217	C	3.369298	-2.88178	-2.34106
O	-1.40118	-2.88392	-1.73433	O	1.746632	-1.11155	-2.51555
O	-1.9185	3.130364	-1.25653	O	-3.85012	-1.86999	-0.50996
O	-0.01209	3.738374	-0.27607	O	-4.19792	0.323799	-0.31958
C	-0.6948	4.817352	0.343299	C	-5.45215	0.046069	0.288752
H	3.556783	-1.68967	-1.9223	H	2.216911	2.225255	0.16136
H	5.56662	-1.24497	-0.50653	H	2.407716	1.021028	-1.98096
H	4.766614	-2.03403	0.878408	H	3.496497	2.425465	-2.01371
H	5.160208	-2.97768	-0.57279	H	1.941535	2.48765	-2.87802
H	2.648724	-3.67022	-0.89104	H	1.55621	4.722601	-1.49919
H	1.39137	-2.41409	-0.79975	H	3.126896	4.413777	-0.71934
H	2.342977	-2.84509	0.643381	H	1.679741	4.665561	0.276802
H	1.824049	-0.21157	-2.35379	H	0.27217	0.789599	-2.14546
H	2.917829	1.400087	0.852101	H	-1.46626	2.610981	0.591561
H	4.244616	0.29001	1.143119	H	-0.50412	4.077542	0.482168
H	1.749376	2.3537	-0.5849	H	-2.41441	1.610346	-0.79509
H	2.784333	-1.35645	2.177239	H	-0.46782	2.951916	2.701323
H	2.604468	0.228871	2.918766	H	1.134832	3.271972	2.041223
H	-3.15846	-1.3562	2.189646	H	2.714246	-0.71403	0.856378
H	-2.06521	-0.30724	3.096337	H	3.019463	-2.17249	1.798769
H	-1.33066	-2.764	1.396562	H	1.785968	-0.93797	3.761257
H	-1.25135	-2.61229	3.127875	H	3.4051	-0.36973	3.331127

H	0.988209	-2.4706	2.282671	H	2.524016	1.753525	2.835162
H	-0.80093	-1.05776	-0.34134	H	0.700739	-0.69122	-0.39143
H	-2.52467	-0.54279	-2.3502	H	-0.52752	-3.40701	-0.79895
H	-2.80724	0.939491	-1.4507	H	-1.396	-2.34257	0.313196
H	-1.16912	1.248078	-3.21415	H	-2.05265	-2.27279	-2.2172
H	-0.18937	-0.10127	-2.6272	H	-0.5837	-1.29897	-2.43898
H	-4.19229	0.273388	0.597481	H	1.450662	-3.93514	1.364661
H	-3.60829	1.209724	2.00304	H	1.067638	-3.29861	2.989667
H	-3.24241	1.775611	0.353106	H	-0.24971	-3.61898	1.832423
H	-3.16422	-4.7565	-1.62299	H	3.087397	-3.94222	-2.33398
H	-4.42411	-3.51653	-1.28213	H	3.689048	-2.57436	-3.34057
H	-3.52883	-4.24616	0.062421	H	4.190706	-2.74984	-1.62371
H	-1.45755	4.432294	1.034081	H	-6.08866	-0.53749	-0.38905
H	0.06106	5.383924	0.894605	H	-5.91165	1.015319	0.50206
H	-1.17933	5.454816	-0.4074	H	-5.30825	-0.52051	1.218188
Conformer 2e (1.55%)							
C	-2.19276	-1.96623	-0.248				
C	-3.56504	-1.35034	-0.52164				
C	-4.67741	-2.32604	-0.13797				
C	-3.75247	0.018943	0.123858				
C	-1.15273	-1.67721	-1.28149				
C	-1.92433	-2.39784	1.193904				
O	-1.85458	-2.91177	-1.24706				
C	0.303264	-1.8084	-1.08934				
C	1.255718	-0.97173	-1.53604				
C	-0.55419	-2.13737	1.829503				
C	-0.12789	-0.67482	1.865053				
C	1.354896	-0.48691	1.68472				
O	1.924	0.653169	1.257785				
C	1.316643	1.937568	1.028856				
C	0.450664	2.355031	2.218283				
C	-0.93575	1.748747	2.280722				
C	-1.03519	0.26651	2.170547				
O	2.10115	-1.41032	1.905114				
C	0.53374	1.843267	-0.29541				
C	1.410482	1.567046	-1.52501				
C	1.029606	0.303009	-2.30453				

C	2.687094	-1.31132	-1.25698
O	-0.15533	3.093889	-0.41865
C	2.492468	2.904375	0.933461
C	-1.23035	3.118396	-1.21894
C	-1.88905	4.466103	-1.22038
O	-1.60692	2.1508	-1.8315
O	3.610193	-0.57678	-1.52204
O	2.856194	-2.5029	-0.68804
C	4.164772	-2.7957	-0.21895
H	-3.60439	-1.21613	-1.61455
H	-4.51704	-3.30396	-0.61451
H	-4.72617	-2.47441	0.951537
H	-5.65382	-1.94024	-0.46408
H	-4.67742	0.483878	-0.24678
H	-2.915	0.691262	-0.11885
H	-3.84494	-0.05617	1.217914
H	-1.47343	-0.99537	-2.07818
H	-2.70205	-1.94358	1.824366
H	-2.12101	-3.48052	1.235334
H	0.620911	-2.72065	-0.58549
H	-0.58896	-2.52187	2.861761
H	0.226954	-2.72691	1.341402
H	0.354438	3.449025	2.199608
H	1.021299	2.102487	3.126223
H	-1.57545	2.173398	1.485778
H	-1.42566	2.055081	3.218391
H	-2.04483	-0.10346	2.364786
H	-0.22348	1.04861	-0.19888
H	1.339762	2.437665	-2.1933
H	2.462665	1.479907	-1.23356
H	1.652459	0.266509	-3.21124
H	-0.01884	0.378661	-2.61739
H	2.14429	3.869208	0.541123
H	2.91944	3.061626	1.933237
H	3.281782	2.511145	0.283011
H	-2.67609	4.489838	-1.97936
H	-1.14204	5.246708	-1.40986
H	-2.32229	4.651592	-0.22754

H	4.438126	-2.08551	0.572436	
H	4.126541	-3.81211	0.183508	
H	4.893399	-2.73506	-1.03723	

Table S3. Conformers of 1*R**,2*S**,7*S**,8*S**-1 for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

conformer	MMFF94 rel. energy	Dihedral angles at MMFF94 level		
	(kcal/mol)	H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0	-114.8	166.8	-78.8
2	0.0503	-115.3	163.8	-81.6
3	0.3797	-115.6	166.3	-79.3
4	0.7148	-116.2	-49.3	64.1
5	0.8867	-114.1	-49.1	64.3
6	1.3223	-125.9	167.2	-79.6
7	1.362	-118.3	176.9	-70.0
8	1.3671	-125.1	168.0	-78.7
9	1.5598	-118.3	178.1	-68.8
10	1.6966	-131.8	-46.6	68.2
11	1.8095	-133.4	-46.6	68.0
12	1.9409	-165.7	-38.8	75.8
13	2.0214	-143.5	-41.7	73.1
14	2.0233	-149.1	-40.1	75.0
15	2.1268	-162.0	-37.8	77.0
16	2.4117	-161.3	-58.1	55.0
17	2.4494	-163.4	-58.2	55.0
18	2.6174	-144.3	-42.1	72.8
19	2.668	-162.6	-58.1	55.1
20	2.6981	-123.9	-175.4	-63.2
21	2.7009	-114.0	177.5	-69.2
22	2.8633	-160.6	-58.3	54.9
23	2.879	-114.5	178.2	-68.6
24	2.9183	-154.6	-174.5	-63.5
25	2.9642	-113.8	162.8	-82.4
26	2.9754	-112.8	160.2	-83.6
27	3.0523	-125.8	-176.4	-64.2
28	3.1159	-126.4	-177.0	-64.9
29	3.1468	-179.8	-168.6	-57.3
30	3.241	-134.6	-61.7	53.0
31	3.2605	-166.8	-172.2	-61.4
32	3.2696	-134.3	-63.0	51.7
33	3.2984	-163.4	-172.8	-61.6
34	3.5209	176.8	-169.5	-58.5
35	3.5798	-135.1	-57.8	56.8
36	3.6432	-115.1	171.7	-73.5
37	3.673	-115.3	-49.3	64.1
38	3.688	-157.5	-173.8	-63.2
39	3.7558	-113.2	159.4	-84.3
40	3.7573	174.8	115.5	-127.8
41	3.7666	-117.4	69.0	-170.7
42	3.8081	-133.1	-60.1	54.5

43	3.8093	-135.8	-62.1	52.5
44	3.834	-113.4	-49.1	64.3
45	3.8767	-115.5	71.1	-168.5
46	3.9137	-111.8	-42.6	71.3
47	3.945	-140.8	-42.5	72.2
48	3.974	-135.8	-61.6	53.1
49	4.049	-135.2	-59.0	55.4
50	4.1323	-154.8	-37.9	77.2
51	4.1586	-136.8	-57.9	56.7
52	4.1639	-124.2	162.5	-82.5
53	4.187	-110.3	-43.1	70.8
54	4.2541	172.7	125.5	-118.8
55	4.3108	-154.9	-37.5	77.5
56	4.3579	-178.5	109.8	-133.1
57	4.3682	-115.2	-176.0	-63.2
58	4.4068	-115.3	171.3	-73.9
59	4.4143	-143.3	-173.6	-62.5
60	4.5492	-158.4	-57.7	55.4
61	4.5578	-121.2	167.6	-79.1
62	4.561	-162.9	-170.7	-59.4
63	4.5633	121.4	167	-79.6
64	4.5845	-142.4	-42.6	72.1
65	4.6488	-160.4	-57.8	55.4
66	4.6702	-128.5	-46.6	68.1
67	4.6751	172.3	132	111.8
68	4.7162	-108.1	-49.3	64.5
69	4.7535	168.7	130.1	-114.4
70	4.762	-116.9	-177.2	-64.5
71	4.7808	-117	-178.1	-65.5
72	4.832	-124.9	162.1	-82.9
73	4.8534	-159.8	-57.6	55.6
74	4.8746	-146.1	-172.8	-62
75	4.9269	-112.7	172.3	-72.8
76	4.9917	-157.8	-57.8	55.3
77	5.0177	-111.3	-49.7	64.2
78	5.0382	-174.7	-38	76.7
79	5.0608	-102	179.3	-67.9
80	5.1246	-133.3	-58	56.7
81	5.2184	172.3	102.6	-139.6

^a Conformers showing dihedral angles over 140° were selected and the vinyl ³J_{H,H} values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.* **1964**, *86*, 5561–5564). ^b Small ³J_{H,H} (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large ³J_{H,H} (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.

Table S4. Conformers of 1*R**,2*S**,7*R**,8*S**-1 for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

conformer	MMFF94 rel. energy (kcal/mol)	Dihedral angles at MMFF94 level		
		H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0	-113.9	80.9	-166.1
2	0.9814	-155.2	79.4	-167.9
3	1.4706	-113.2	92.9	-152.3
4	1.4913	171.1	80.8	-166.2
5	1.5453	173.6	79.8	-167.1
6	1.8883	-114.7	-70.7	44.2
7	2.053	-135.1	83.8	-161.0
8	2.0937	-114.4	-70.7	44.2
9	2.1401	-114.3	-72.0	42.7
10	2.1944	173.7	83.2	-163.4
11	2.3006	176.7	82.3	-164.1
12	2.3032	-156.2	170.4	-71.9
13	2.351	-115.2	90.4	-155.1
14	2.4791	-125.4	-69.0	45.0
15	2.4832	-119.3	67.3	-179.8
16	2.6149	-125.5	-69.8	44.0
17	2.6744	-115.2	-71.2	43.6
18	2.6946	-164.5	63.9	175.5
19	2.7274	-136.7	83.9	-160.9
20	2.7659	-117.3	67.9	-179.2
21	2.7673	-162.6	63.7	175.2
22	2.9523	-156.3	170.1	-72.2
23	2.9854	-117.4	-62.9	51.6
24	2.9946	-125.7	-68.7	45.1
25	3.0161	-113.6	80.8	-166.3
26	3.0242	-162.4	62.7	174.0
27	3.086	-164.4	62.8	174.1
28	3.216	-140.0	89.5	-154.6
29	3.3279	-117.1	-64.0	50.3
30	3.3957	-118.3	67.9	-179.2
31	3.5471	-150.9	171.9	-70.2
32	3.9464	-147.5	161.6	-80.1
33	4.0261	-154.3	89.6	-154.8
34	4.034	-114.3	79.4	-167.9
35	4.1515	173.4	81.7	-165.2
36	4.1673	177.1	81.8	-164.8
37	4.2281	-127.2	-58.3	55.7
38	4.2555	-151.2	171.9	-70.3
39	4.2844	-114.0	-62.6	52.1
40	4.2935	-126.8	-58.3	55.7
41	4.2945	-152.6	-54.3	58.2
42	4.4039	-126.5	-58.9	55
43	4.4687	-107.1	63.4	176.3

44	4.4815	-128.4	170.6	-71.1
45	4.6474	-147.2	161.4	-80.4
46	4.6558	-113.4	-63.6	50.8
47	4.6958	-156.4	89.6	-154.8
48	4.7279	-126.1	-57.7	56.2
49	4.739	-161.3	92.4	-152
50	4.7794	-113.4	-71.3	43.6
51	4.8287	-133.4	58.2	170.6
52	4.9241	-150.6	-53.9	58.6
53	4.9568	-113.1	-71.3	43.5
54	4.9728	-161.3	64.2	175.9
55	4.9746	-113.9	82.3	-163.2
56	4.9922	-159.6	64.0	175.6
57	5.0376	-113.0	-72.6	42.1
58	5.0705	-150.1	-53.3	59.3
59	5.1581	-107.8	63.5	176.4
60	5.2551	-159.2	63.1	174.4
61	5.3019	-161.4	-51.5	61.4
62	5.3488	-128.4	171.3	-70.5
63	5.3763	-161.1	63.2	174.6
64	5.4268	-134.5	57.2	169.6
65	5.4512	-134.6	58.3	170.6

^a. Conformers showing dihedral angles over 140° were selected and the vinyl ³J_{H,H} values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.* **1964**, *86*, 5561–5564). ^b. Small ³J_{H,H} (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large ³J_{H,H} (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.

Table S5. Conformers of 1*R**,2*S**,7*S**,8*R**-1 for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

conformer	MMFF94 rel. energy	Dihedral angles at MMFF94 level		
	(kcal/mol)	H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0	-176.9	176.3	-71.5
2	1.019	-179.4	177.0	-71.0
3	2.7493	-169.4	176.9	-71.0
4	3.887	-154.9	-38.1	77.0
5	3.8955	-172.0	178.3	-69.8
6	3.9172	-161.7	177.8	-69.9
7	4.0306	-155.7	-37.7	77.6
8	4.0672	-158.3	-36.7	78.4
9	4.43	-157.0	-38.0	77.1
10	4.643	-165.4	171.1	-70.2
11	4.832	-177.7	171.0	-75.0
12	5.1697	-174.8	170.9	-75.4
13	5.6161	-179.3	67.2	-177.4
14	6.2459	-176	66.5	-177.7

^a. Conformers showing dihedral angles over 140° were selected and the vinyl ³*J*_{H,H} values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.* **1964**, 86, 5561–5564). ^b. Small ³*J*_{H,H} (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large ³*J*_{H,H} (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.

Table S6. Conformers of 1*R**,2*S**,7*R**,8*R**-1 for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

conformer	MMFF94 rel. energy (kcal/mol)	Dihedral angles at MMFF94 level		
		H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0	-173.3	-56.8	56.4
2	1.1514	-168.8	-56.3	56.9
3	2.1387	-154.4	87.6	-156.8
4	2.2075	-157.8	91.5	-152.5
5	2.4439	-157.5	92.5	-151.5
6	2.4895	-168.7	-56.7	56.5
7	3.4132	-164.8	-56.1	57.1
8	4.2175	-154.3	91.6	-152.3
9	4.5219	-147.9	82.5	-162.7
10	4.5525	-149.4	85.0	-159.9
11	4.5605	-154.1	88.6	-156.5
12	4.595	-152.6	87.3	-157.1
13	4.748	-152.8	88.5	-156.6
14	4.9092	-148.1	82.5	-162.7
15	5.049	-150.8	87.6	-157.4
16	5.2953	-124.6	-47.9	67.1
17	5.3583	-124.1	-49.2	65.7

^a. Conformers showing dihedral angles over 140° were selected and the vinyl ³*J*_{H,H} values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.* **1964**, *86*, 5561–5564). ^b. Small ³*J*_{H,H} (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large ³*J*_{H,H} (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.

Table S7. Conformers of 1*R**,2*R**,7*R**,8*R**-2 for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

conformer	MMFF94 rel. energy	Dihedral angles at MMFF94 level		
	(kcal/mol)	H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0	72	150.2	-94.3
2	0.1034	87.5	-56.6	56
3	0.3151	75.6	153.3	-91.6
4	0.4103	82.9	-53.9	58.6
5	0.6114	71.1	154.9	-90
6	0.8517	71.5	149.1	-95.3
7	0.8883	69.8	154.1	-90.7
8	1.0333	-149.8	-44.8	67.8
9	1.1472	75	153.3	-91.6
10	1.2774	73.5	156.7	-88.5
11	1.2915	-147.5	141.9	-102.4
12	2.1929	-147.1	145.8	-98.8
13	2.3801	76.5	-50.6	61.9
14	2.5059	-148.3	141	-103.3
15	2.5459	87.1	-58	54.6
16	2.5487	91.5	92.8	-149.3
17	2.5749	-147.6	-47.2	65.4
18	2.5866	72.8	150.7	-94.2
19	2.6492	94.5	-173.5	-62.6
20	2.7529	92.3	92.3	-149.7
21	2.8419	-150.1	-44	68.6
22	2.9572	-144.5	144.5	-100.1
23	3.1574	93.4	-173.1	-62.3
24	3.2239	-148.3	144.7	-99.9
25	3.314	71.5	85.8	-156.9
26	3.3628	72.3	151.6	-93.4
27	3.5767	91.8	-57.5	55.2
28	3.5775	70.6	86.2	-156.6
29	3.7057	-144.4	148.7	-96.3
30	3.792	99.1	119.4	-124.5
31	3.811	99.7	119.4	-124.5
32	3.8688	91.3	91.8	-150.3
33	3.9242	92.9	114	-129.6
34	4.0816	92.2	91.4	-150.7
35	4.0923	-157.5	134.2	-110
36	4.1074	93.9	113.2	-130.3
37	4.1878	88.2	76.9	-166
38	4.2035	-134.1	-163.7	-52.9
39	4.2136	-135.3	-165.4	-54.7
40	4.2488	73.3	65.7	-179.4
41	4.3504	97.3	79.2	-163.4
42	4.3603	88.9	-177.9	-66.8
43	4.4019	-147.8	-46.8	65.8

44	4.4057	79.7	155.4	-88.8
45	4.4064	-155.4	133.3	-110.9
46	4.4222	-155.3	-40.4	72.5
47	4.4891	-144	140.6	-103.7
48	4.5187	65.6	70.4	-173.6
49	4.5397	-142.1	-57.2	55.4
50	4.5454	86.5	73.1	-170
51	4.5741	87.6	77.7	-165.2
52	4.6065	76.1	150.5	-92.9
53	4.6174	96.5	79.5	-163
54	4.6227	-153.4	-43.3	69.6
55	4.6687	-127.4	-165.8	-55.6
56	4.6741	78.1	155	-89.1
57	4.71	-143.4	-56.9	55.8
58	4.7423	-133.4	-163.8	-52.9
59	4.7507	-154.4	-42	71
60	4.7661	-134.6	-165.6	-54.8
61	4.8225	74.6	150.3	-93
62	4.9011	85.8	73.6	-169.5
63	4.9217	65.7	68.7	-175.5
64	4.9465	-155.1	132.4	-111.3
65	5.0236	-155.8	-43.7	69.1
66	5.0359	-143	-56.8	55.9
67	5.0435	101.8	118.4	-128.4
68	5.061	-144.2	144.5	-100
69	5.0817	102.3	118.4	124.8
70	5.0985	-141.8	-57.4	55.2
71	5.1677	-125.6	-164.4	-54.1
72	5.2277	81.8	-57	55.9
73	5.2449	71.2	74.9	-168
74	5.2477	82.4	-56.7	56.1
75	5.2605	99.5	118.5	-125.2
76	5.2958	100.2	118.6	-125.1
77	5.3744	93.8	93.3	-148.8
78	5.3913	96.4	77.1	-165.5
79	5.4288	-151.2	134.1	-108.2
80	5.4354	-158.2	137.4	-106.9
81	5.4552	-155.5	134.8	-109.1
82	5.4756	92.9	112.8	-130.8
83	5.488	77.2	87.9	-154
84	5.4976	-132.5	-164.5	-53.6
85	5.5055	-133.8	-165.9	-55.1
86	5.5131	71.3	75.4	-167.3
87	5.5553	-155.7	133.5	-110.6
88	5.5801	94.6	92.8	-149.3
89	5.5916	94.7	-67.5	45.1
90	5.5973	74.1	80	-161.6
91	5.6104	71.1	84.6	-158
92	5.6428	98.2	-172.4	-61.5

93	5.6484	95.5	77.4	-165.2
94	5.6662	93.9	111.9	-131.5
95	5.7065	77.4	88.3	-153.4
96	5.7741	74.4	80.6	-160.9
97	5.8439	75	62.9	177.5
98	5.8592	101	103.8	-139.1
99	5.8785	70.2	85.1	-157.6
100	6.0457	101.1	103.6	-139.3

^a. Conformers showing dihedral angles over 140° were selected and the vinyl ³J_{H,H} values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.* **1964**, 86, 5561–5564). ^b. Small ³J_{H,H} (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large ³J_{H,H} (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.

Table S8. Conformers of 1*R**,2*R**,7*S**,8*R**-**2** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

conformer	MMFF94 rel. energy (kcal/mol)	Dihedral angles at MMFF94 level		
		H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0	-147.9	81.3	-166.1
2	1.4734	-145.2	79.9	-167.9
3	1.5167	-146.4	90.8	-156.3
4	1.8714	-148.1	81.7	-165.6
5	2.6284	-147.4	-89	24.5
6	2.7953	-138	147.4	-95.7
7	3.3378	-142	66.1	177.3
8	3.356	-111.9	173.9	-68.5
9	3.4379	-145.5	77.8	-170
10	3.4861	-143.4	66.6	178
11	3.5591	-141.7	64.7	175.6
12	3.8114	-143.1	65.1	176.2
13	3.8997	-141.1	115.6	-128.2
14	4.1878	-112	174.5	-68
15	4.2191	-156.7	-93.8	19.4
16	4.2554	-144.7	144.7	-98.3
17	4.3661	-147.6	121.6	-121.7
18	4.3748	-143.7	-86.7	26.6
19	4.7025	-156.2	-96.2	17.1
20	4.7456	-153.1	86.3	-160.2
21	4.828	-150.4	147.1	-95.8
22	5.0198	-143.6	-86.9	26.7
23	5.037	-133.9	155.9	-86.8
24	5.0635	-152.5	83.8	-162.8
25	5.4057	-148.4	85.4	-160.4
26	5.454	-149.2	-87.2	26.3
27	5.4741	-153	79.4	-167.9
28	5.521	-151.7	146	-96.7
29	5.5485	-141.7	64.7	175.7
30	5.6026	-144.7	145.4	-98
31	5.6295	-143	65.2	176.4
32	5.6586	-156.1	-91.5	21.7
33	5.6598	-141.4	63.5	174.2
34	5.7175	-150.1	148.2	-94.8
35	5.8477	-142.8	63.8	174.7
36	5.8509	-141.3	64.8	175.8
37	5.9047	-148.8	-88.1	25.4
38	5.9216	-142.6	65.2	176.4
39	5.9331	-141	63.6	174.2
40	5.9465	-106.9	171.4	-70.8
41	6.0556	-132.9	159.1	-83.6

^a. Conformers showing dihedral angles over 140° were selected and the vinyl ³*J*_{H,H} values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.*

1964, 86, 5561–5564). ^b. Small $^3J_{\text{H,H}}$ (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large $^3J_{\text{H,H}}$ (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.

Table S9. Conformers of 1*R**,2*R**,7*R**,8*S**-2 for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (the selected conformers were marked in yellow).

conformer	MMFF94 rel. energy (kcal/mol)	Dihedral angles at MMFF94 level		
		H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0.000	-147.6	-178.8	-66.8
2	0.204	-150.3	-177.7	-65.7
3	1.726	-138.3	65.3	-177.4
4	2.220	-145.2	178.7	-69.1
5	2.593	-148.6	-179.1	-66.9
6	4.093	-140.4	69	-173.6
7	4.444	-136.4	67.4	-174.9
8	4.795	-149.1	174.7	-71.5
9	4.968	-169.1	113.4	-130.2
10	5.042	-147.4	174.2	-72.1
11	5.2739	-150.1	-50.7	61.9
12	5.6045	-148.5	-50.8	61.8
13	5.871	-143.0	60.9	176.6

^a. Conformers showing dihedral angles over 140° were selected and the vinyl $^3J_{\text{H,H}}$ values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.* 1964, 86, 5561–5564). ^b. Small $^3J_{\text{H,H}}$ (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large $^3J_{\text{H,H}}$ (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.

Table S10. Conformers of 1*R**,2*R**,7*S**,8*S**-**2** for *J*-DP4 calculation and the dihedral angles of selected protons at MMFF94 level (none of the conformers was selected).

conformer	MMFF94 rel. energy	Dihedral angles at MMFF94 level		
	(kcal/mol)	H-2/H-3 ^a	H-7/H-6 <i>pro-R</i> ^b	H-7/H-6 <i>pro-S</i> ^b
1	0.000	72	103.8	-140.8
2	0.137	87.5	-72.9	39.4
3	0.442	75.6	122.9	-121.1
4	0.513	82.9	106.5	-138.1
5	0.664	71.1	-73.6	38.6
6	0.772	71.5	101	-143.8
7	0.916	69.8	105.5	-139.1
8	1.175	75	103.7	-140.9
9	1.290	73.5	109.8	-134.7
10	1.601	-147.5	-73.2	38.9
11	1.685	-147.1	103.2	-141.5
12	1.969	76.5	108.8	-135.5
13	2.022	-148.3	-74.3	37.7
14	2.052	87.1	125.5	-118.7
15	2.428	91.5	124.3	-119.5
16	2.461	-144.5	55.6	166.1
17	2.517	93.4	123.8	-120.1
18	2.553	-148.3	155.7	-86.8
19	2.858	71.5	53.4	164.1
20	2.996	72.3	56.1	166.6
21	2.997	91.8	111.9	-132.9
22	3.282	70.6	56.1	166.4
23	3.284	-144.4	114	-130.8
24	3.344	99.1	-176.6	-60.2
25	3.413	99.7	54	164.8
26	3.484	91.3	110.1	-134.7
27	3.643	92.9	143	-99.5
28	3.660	92.2	-174.2	-58.3
29	3.893	-157.5	105	-139.7
30	3.938	93.9	113	-131.5
31	3.961	88.2	111.7	-133.1
32	4.039	-134.1	-79.6	32.9
33	4.081	-135.3	127.5	-116.6
34	4.081	73.3	99.8	-145
35	4.095	97.3	111.2	-133.1
36	4.115	88.9	152.5	-89.5
37	4.142	79.7	126.6	-117.6
38	4.154	-155.4	54.8	165.2
39	4.165	-144	143.6	-99
40	4.254	65.6	56.6	166.9
41	4.490	86.5	114.1	-130.2
42	4.586	87.6	-177.3	-60.8
43	4.590	76.1	155.7	-86.7
44	4.593	96.5	-77.1	35.5

45	4.619	-127.4	141.6	-100.8
46	4.624	78.1	113	-129.5
47	4.627	-133.4	155.6	-86.9
48	5.108	-134.6	-171.1	-55
49	5.1161	73	55.6	166
50	5.1945	74.6	142	-100.4
51	5.3231	94.2	117.2	-125.2
52	5.3364	90.3	-174.4	-57.9
53	5.406	90	-176.3	-59.8
54	5.6019	101	-73.5	39.5
55	5.6615	69.7	-174.1	-58.3
56	5.6656	87.6	59.3	171.3
57	5.692	68.5	-72.1	40.1
58	5.786	73.3	-65.4	48.9
59	5.8481	72.7	-64.9	49.2
60	5.8582	99	-72.1	41.1
61	5.9031	70.4	-66.7	45.7
62	5.9453	69.4	44.6	-67.8

^a. Conformers showing dihedral angles over 140° were selected and the vinyl $^3J_{\text{H,H}}$ values can be estimated using the modified Karplus Equation by Garbisch (Garbisch, E. W., Jr. *J. Am. Chem. Soc.* **1964**, 86, 5561–5564). ^b. Small $^3J_{\text{H,H}}$ (< 4 Hz) values were selected based on dihedral angles in the range 50–120° and large $^3J_{\text{H,H}}$ (> 8 Hz) values were in the ranges 0–30° and /or 140–180°.