Supplementary Informations

Bio-inspired benzo[*k,l*]xanthene lignans: synthesis, DNA-interaction and antiproliferative properties

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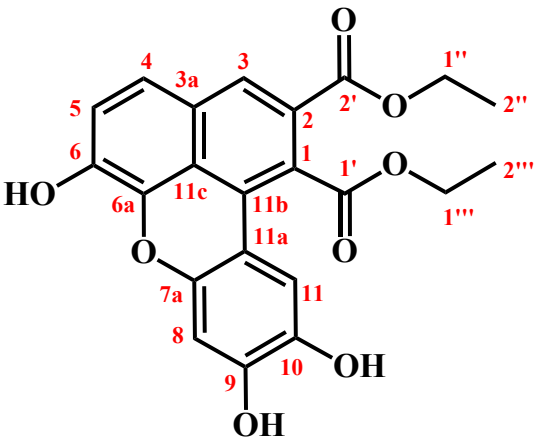
Contents of Supplementary Informations



27

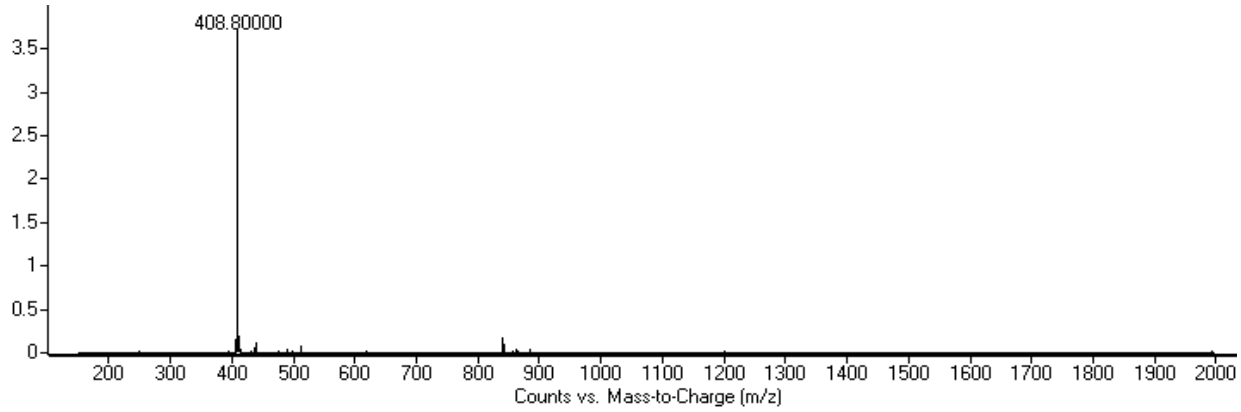


Figure 1S: ESI-MS spectrum of **27**

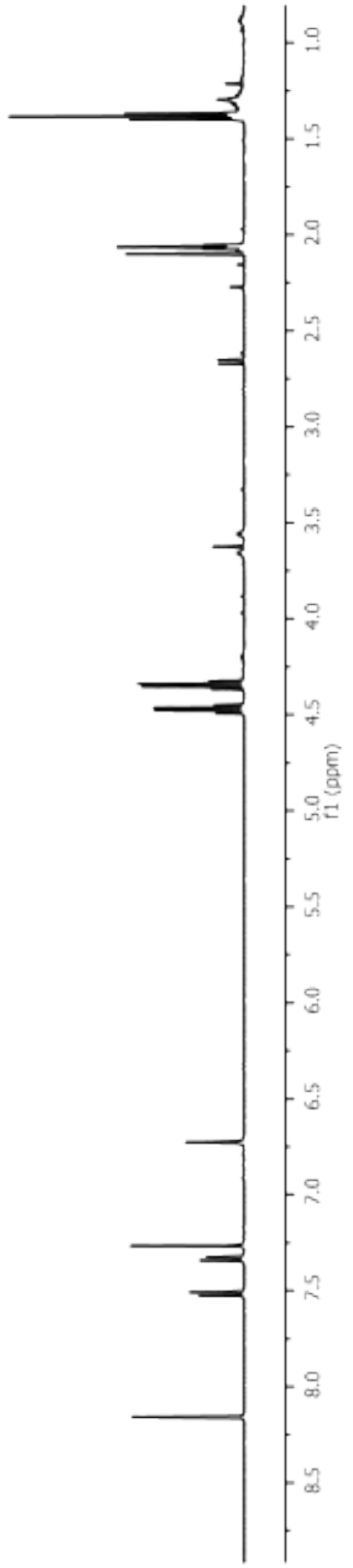


Figure 2S: ^{1}H-NMR spectrum (CD_3COCD_3, 500 MHz) of **27**

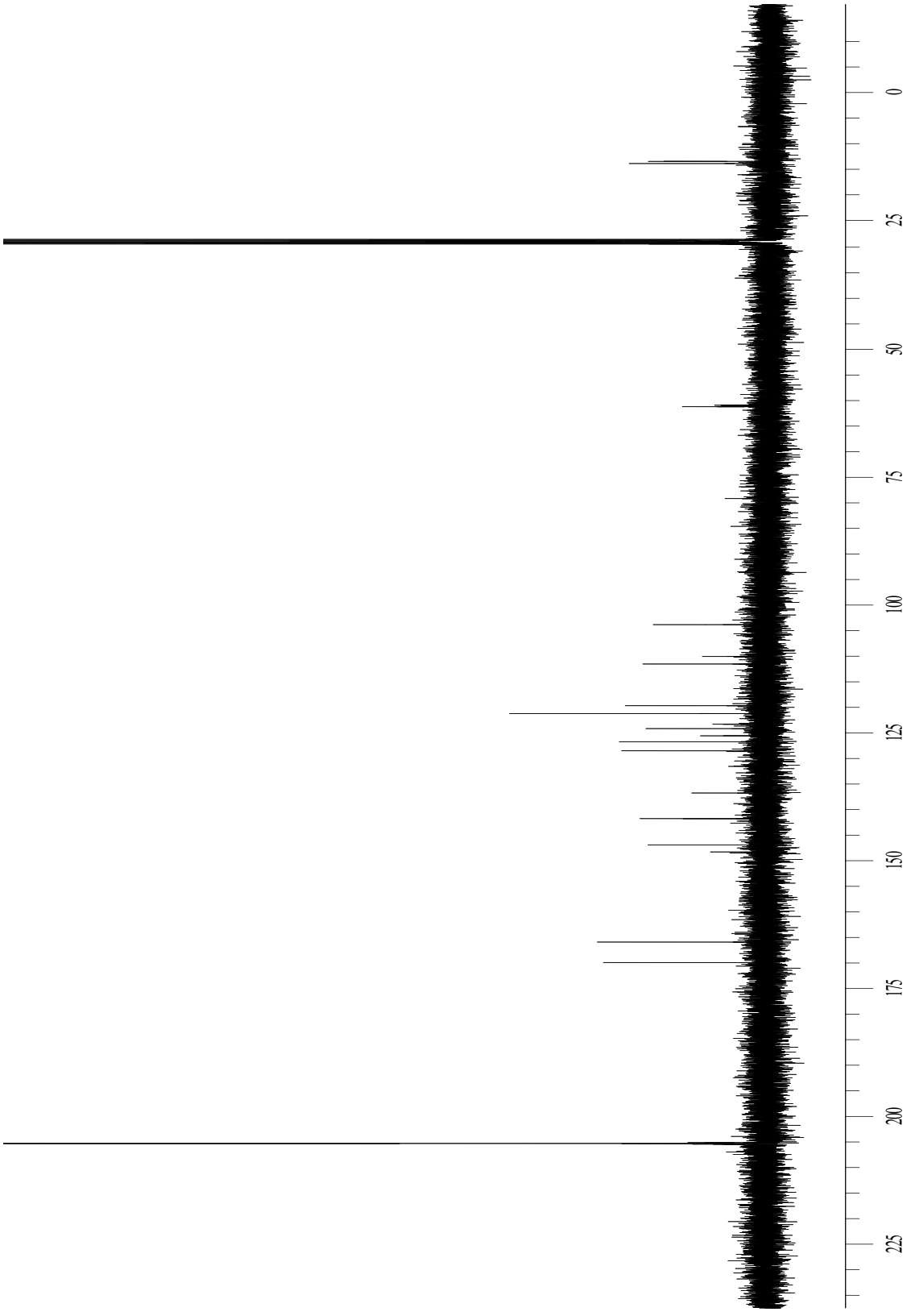
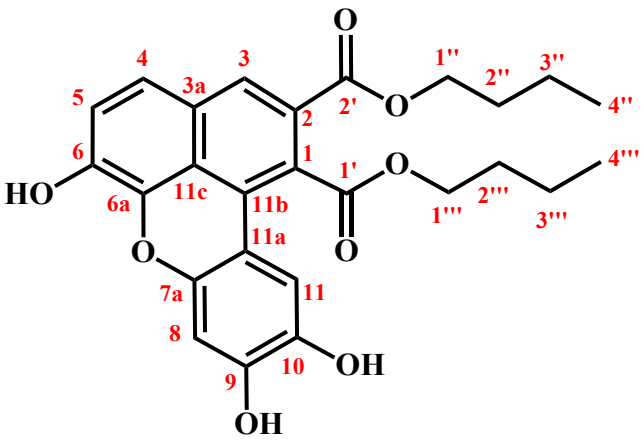


Figure 3S: ^{13}C- NMR spectrum (CD_3COCD_3, 125 MHz) of **27**



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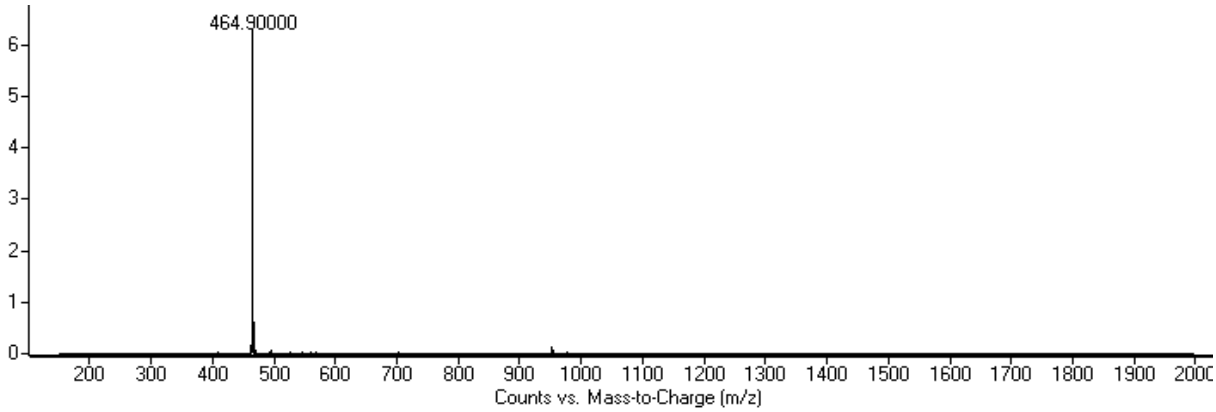


Figure 4S: ESI-MS spectrum of **28**

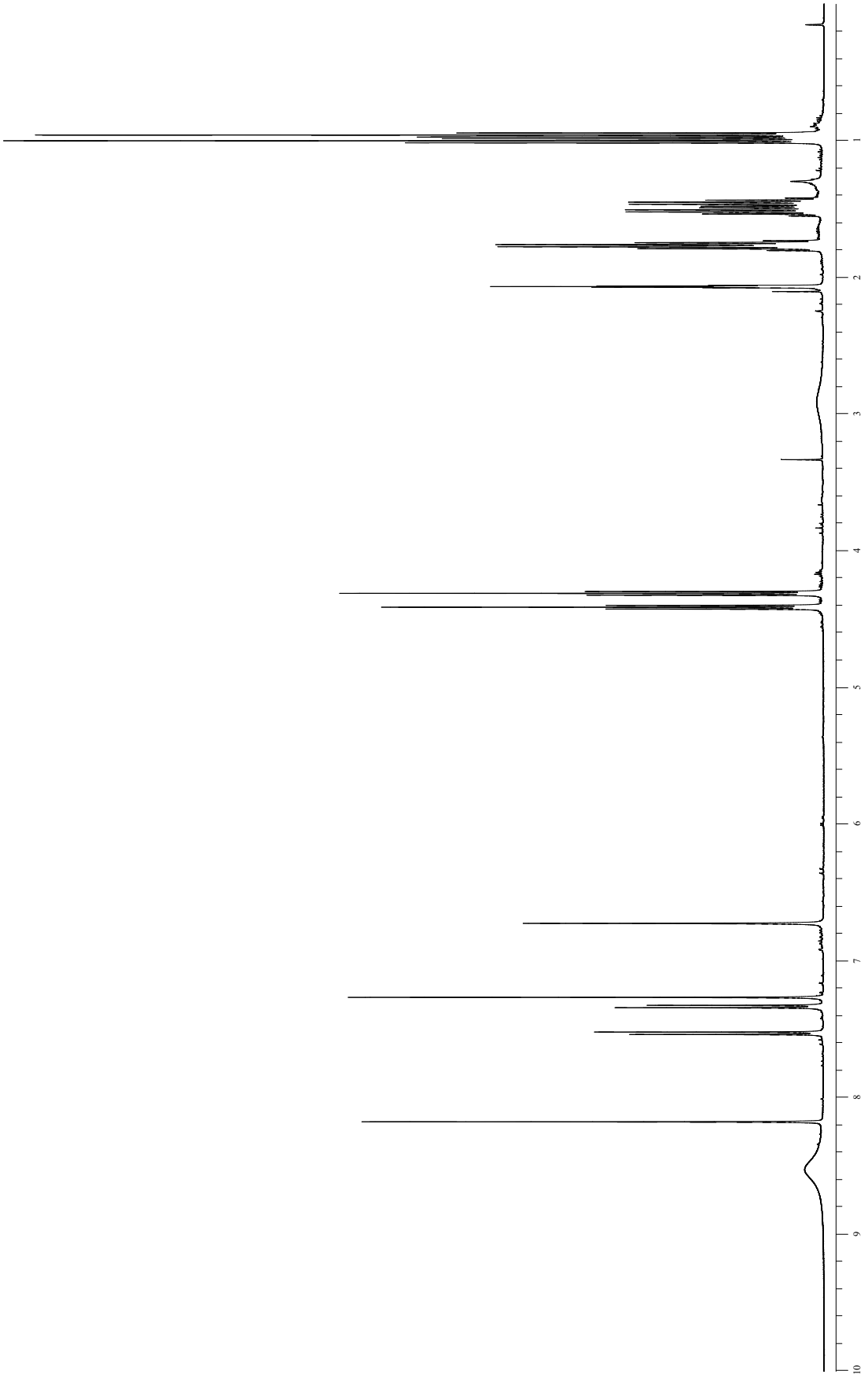


Figure 5S: ^{1}H-NMR spectrum (CD_3COCD_3, 500 MHz) of **28**

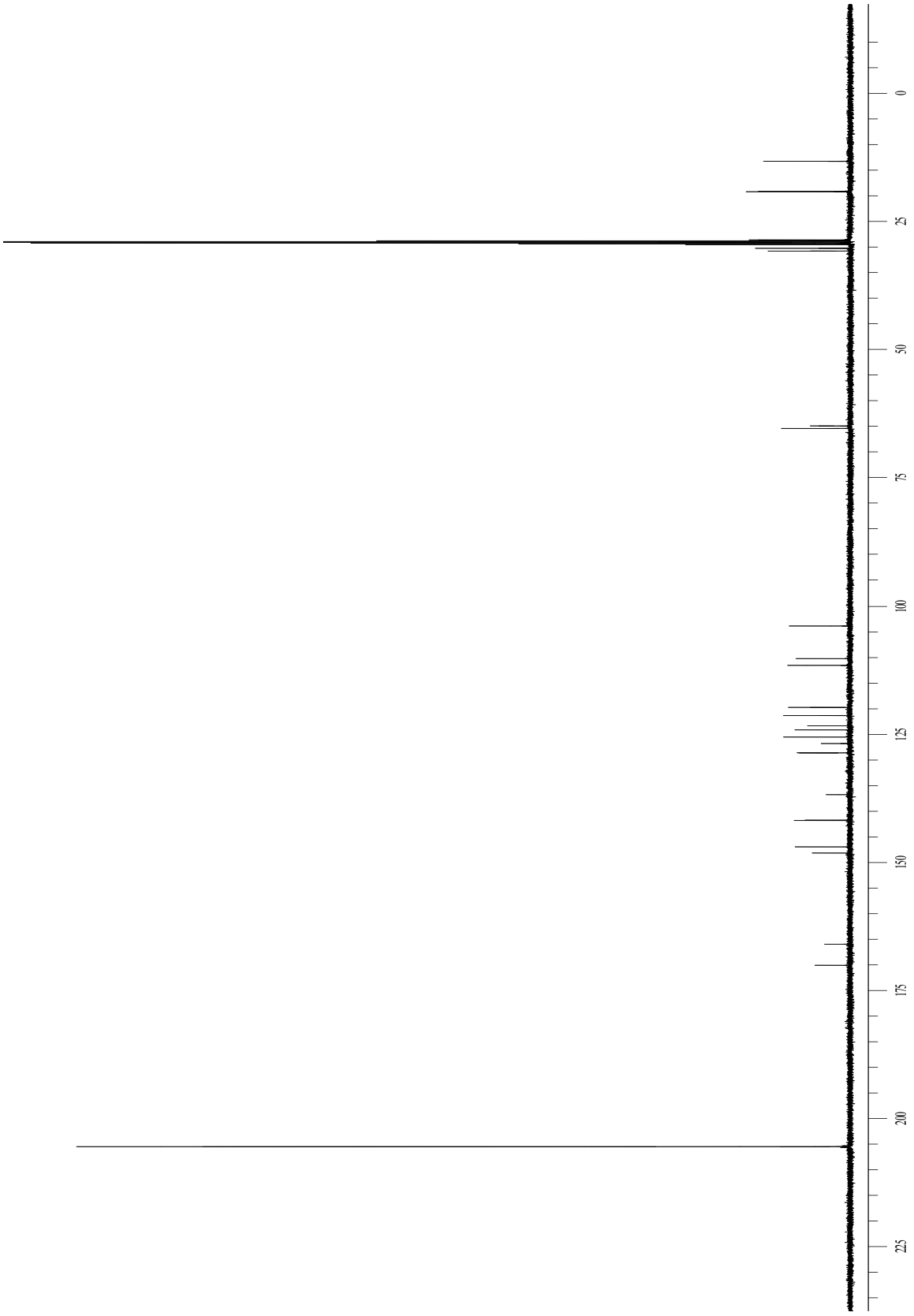
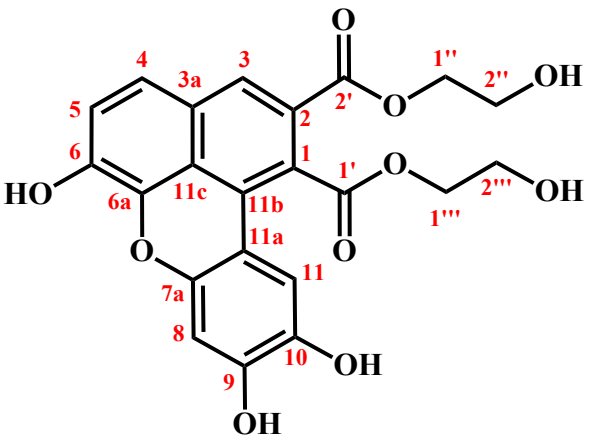


Figure 6S: ^{13}C- NMR spectrum (CD_3COCD_3, 125 MHz) of **28**



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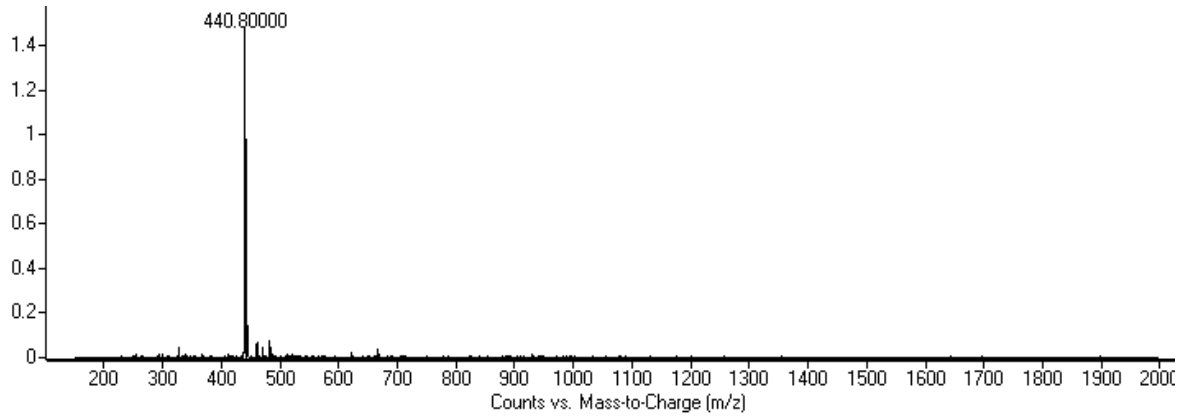


Figure 7S: ESI-MS spectrum of **29**

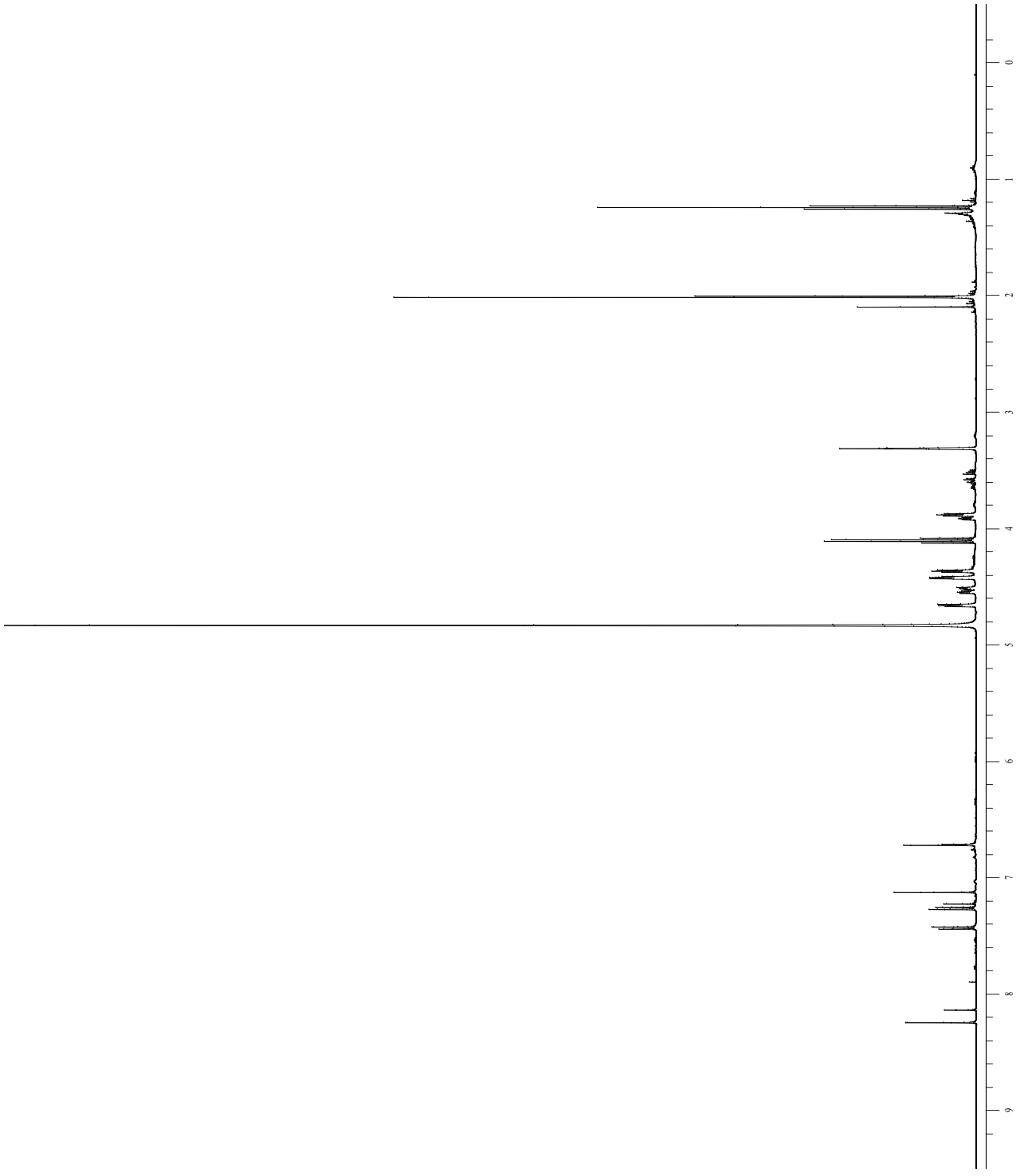


Figure 8S: ^{1}H-NMR spectrum (CD_3COCD_3, 500 MHz) of **29**

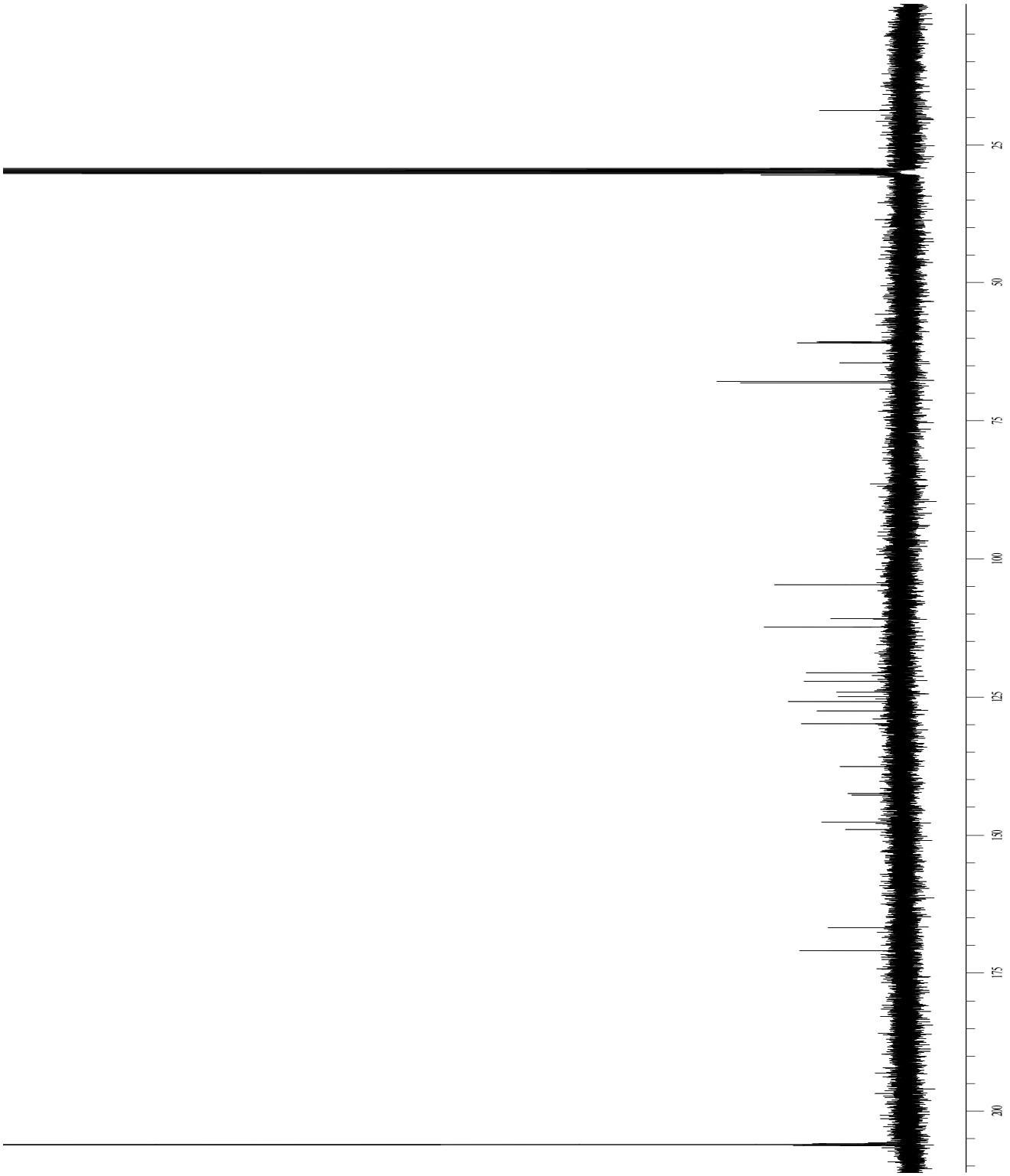
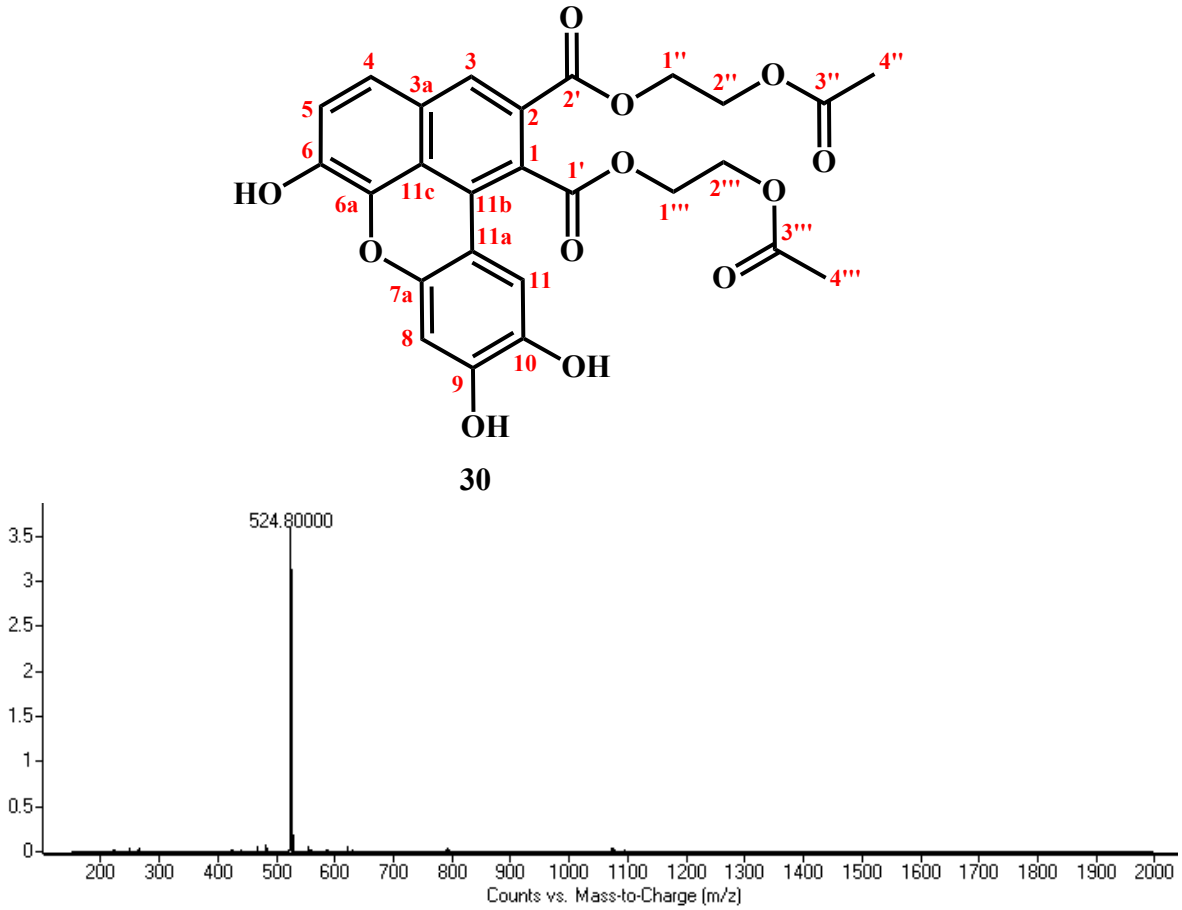


Figure 9S: ^{13}C- NMR spectrum (CD_3COCD_3, 125 MHz) of **29**



30

Figure 10S: ESI-MS spectrum of **30**

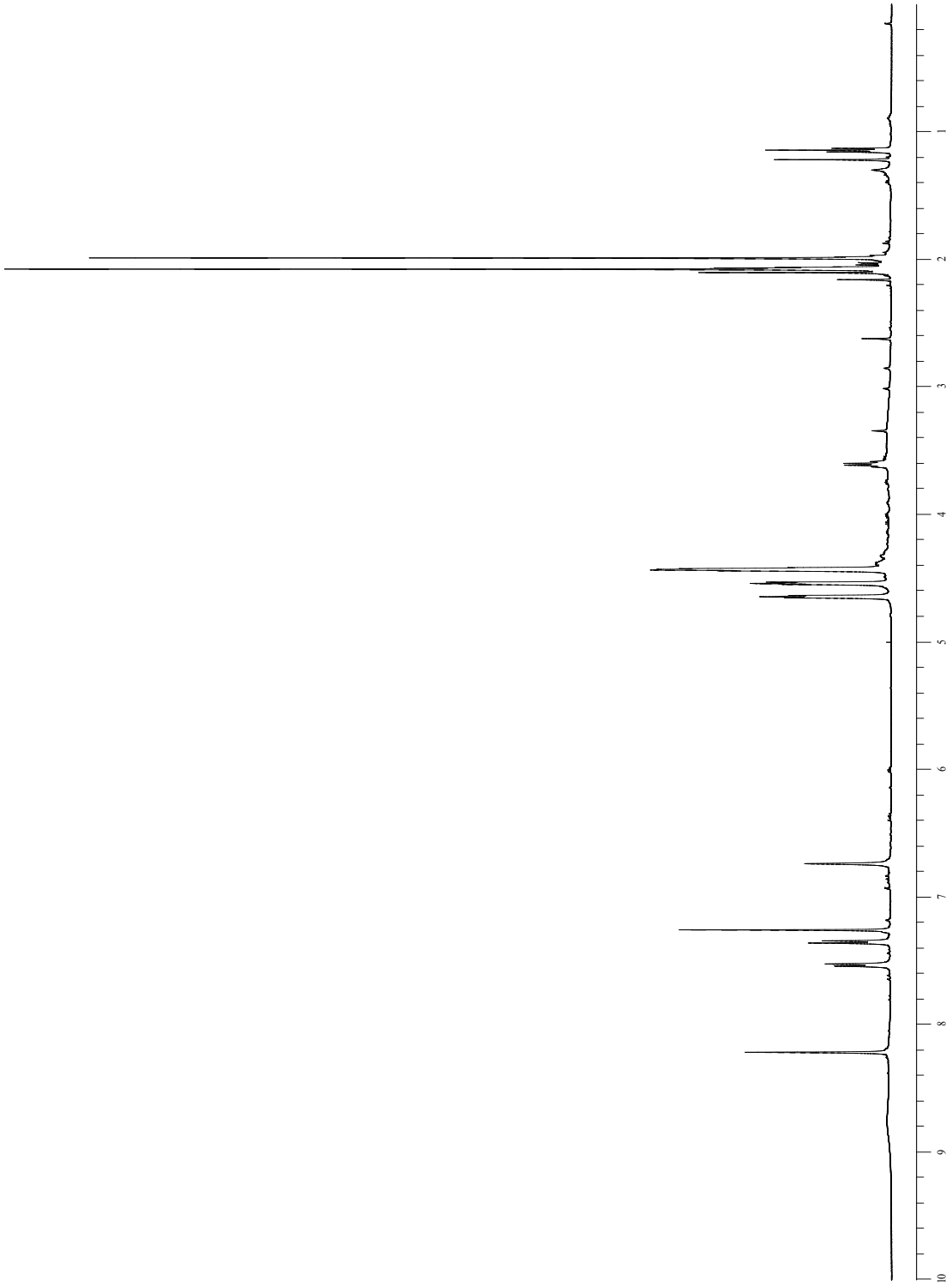


Figure 11S: ^{1}H-NMR spectrum (CD_3COCD_3, 500 MHz) of **30**

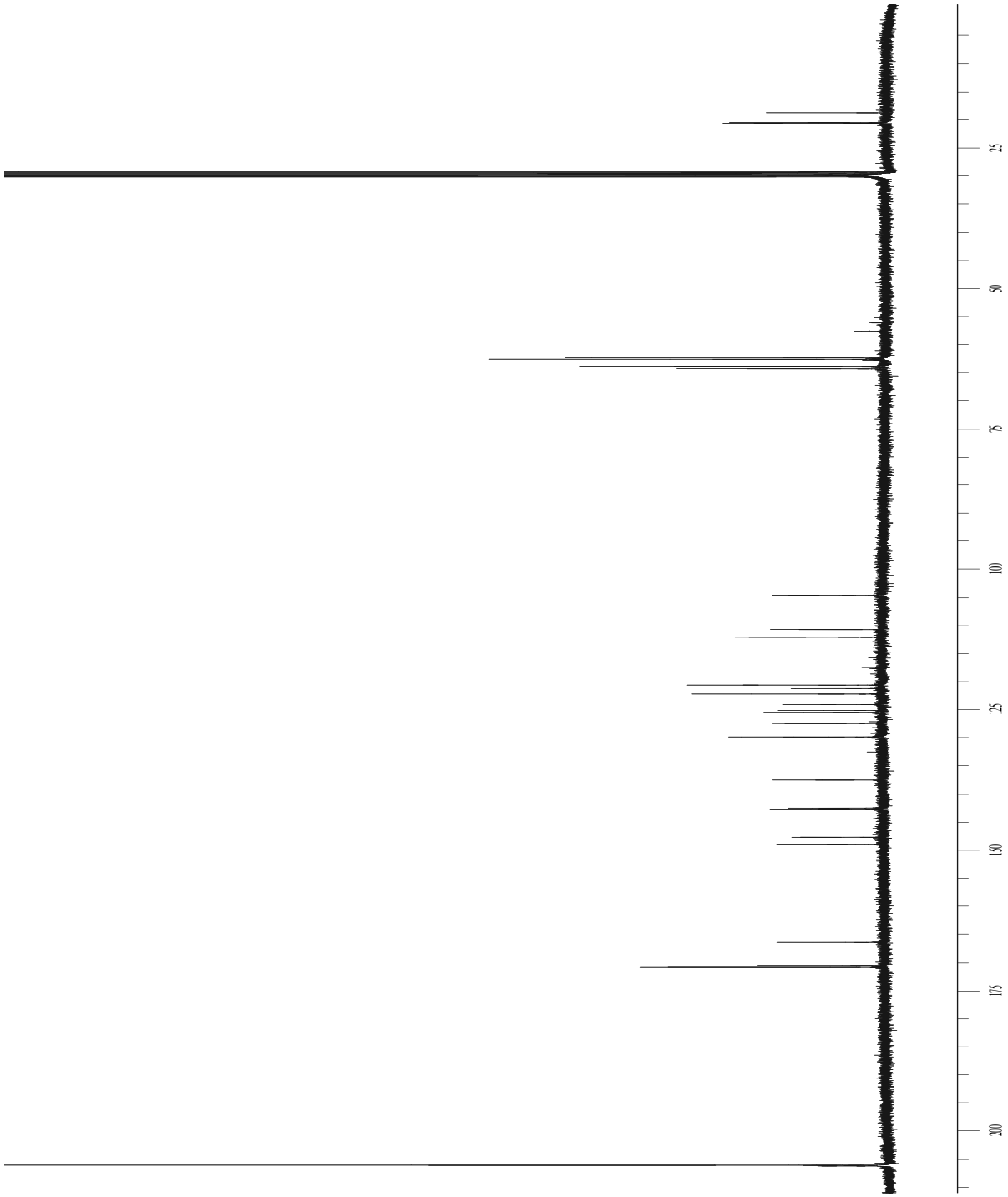


Figure 12S: ^{13}C- NMR spectrum (CD_3COCD_3, 125 MHz) of **30**

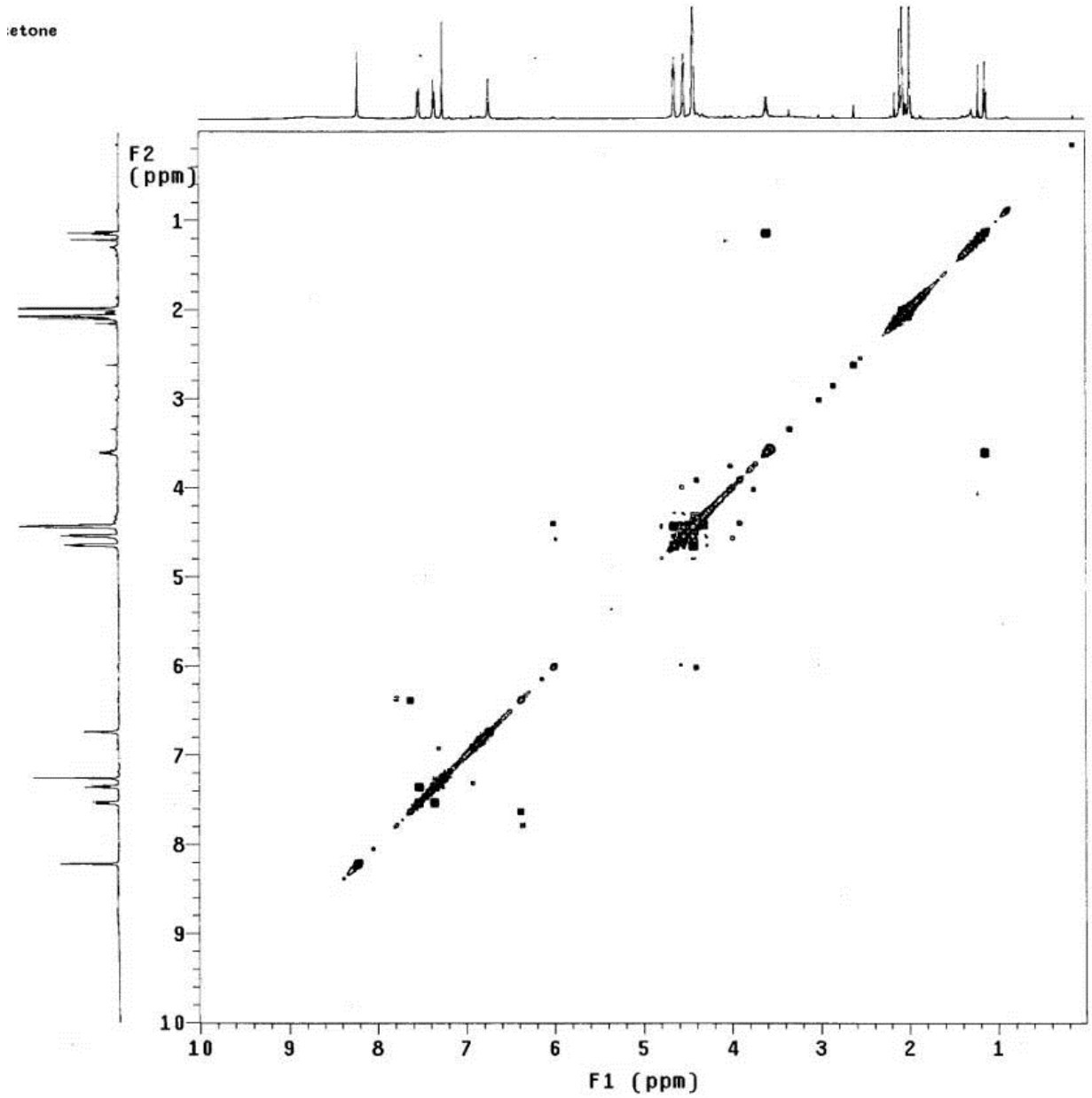
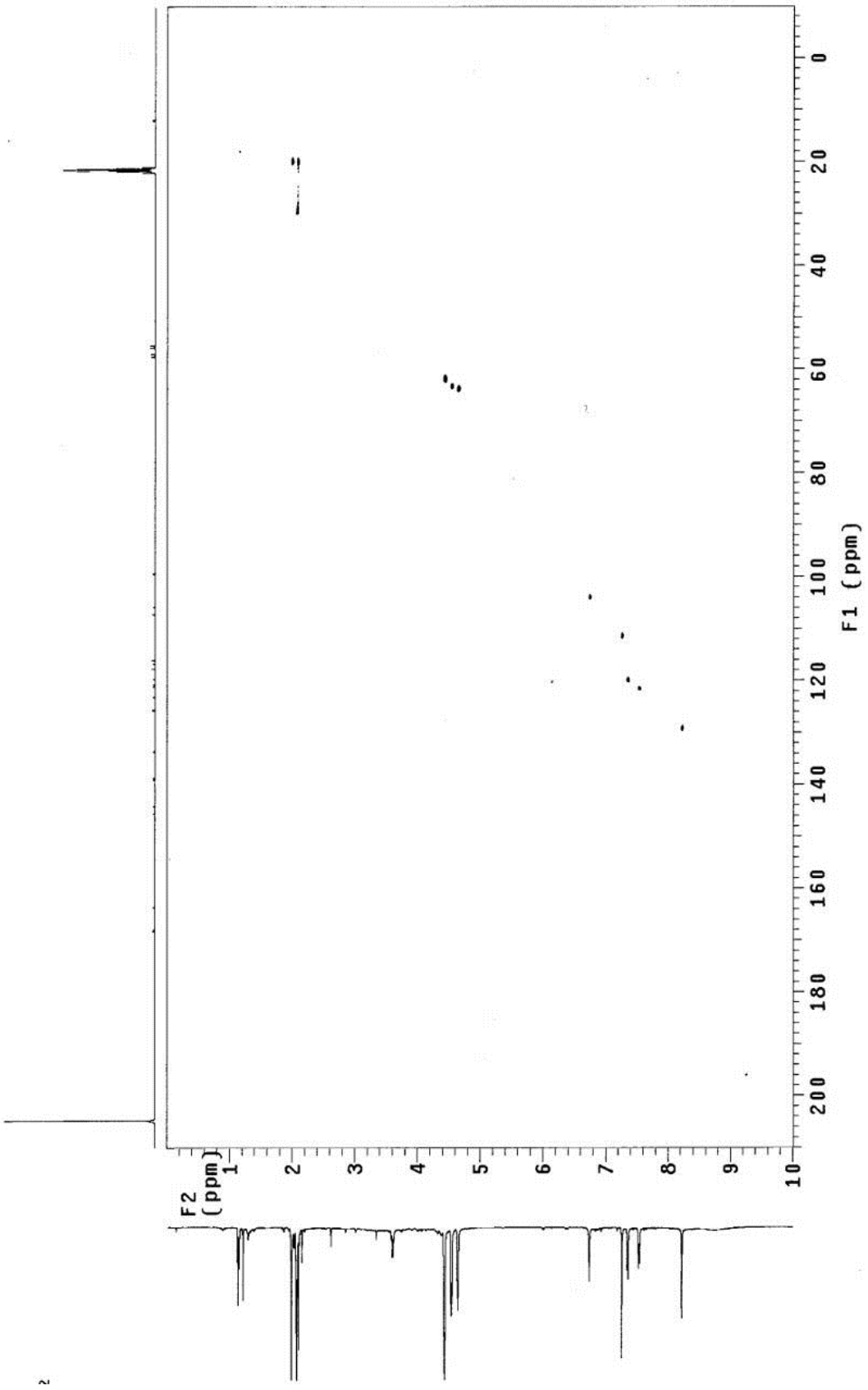


Figure 13S: COSY spectrum (CD_3COCD_3, 500 MHz) of **30**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3
4
5
6
7
8
9
10
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60
80
100
120
140
160
180
200

Figure 14S: HSQC spectrum (CD_3COCD_3, 500 MHz) of **30**

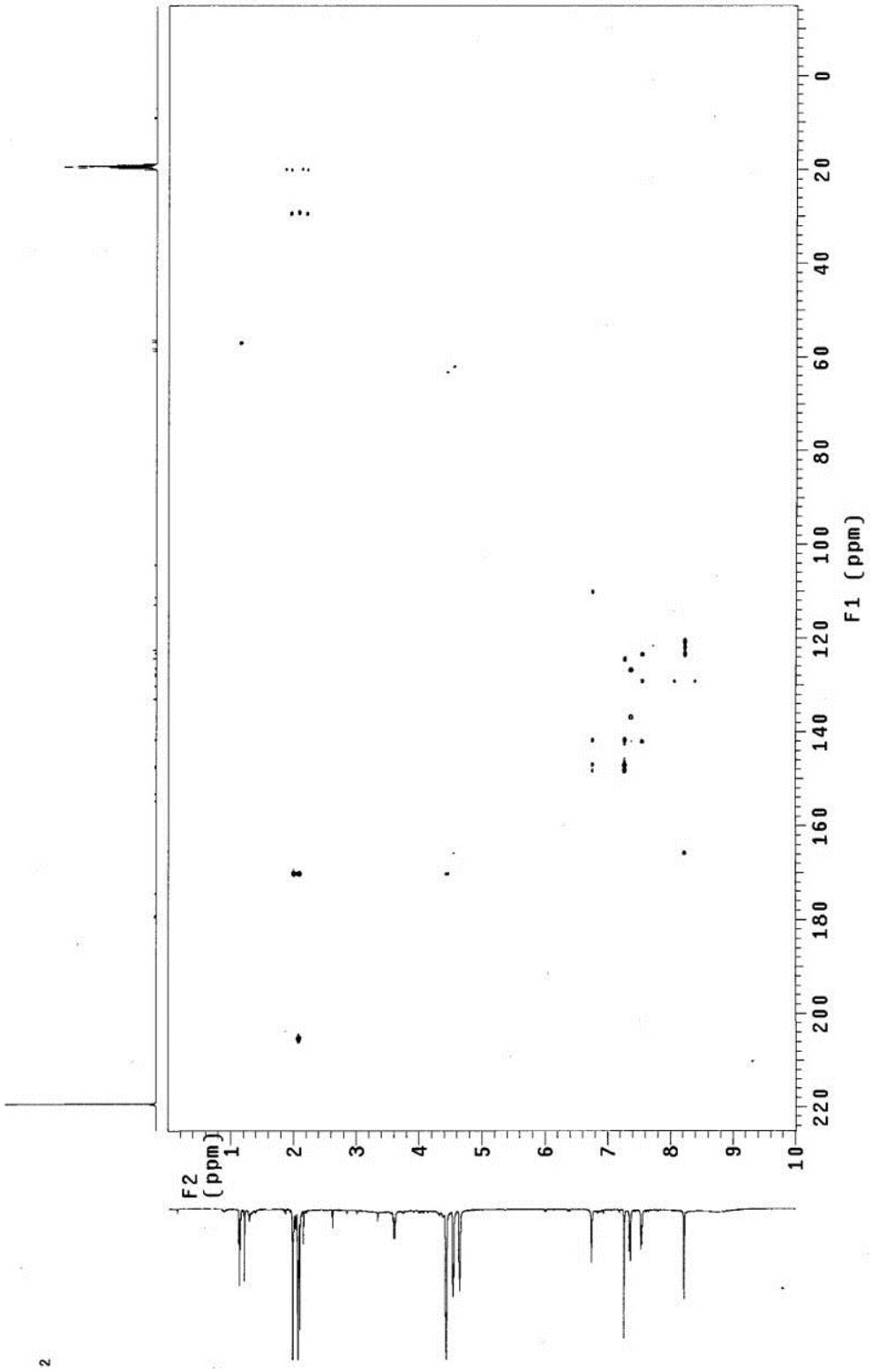
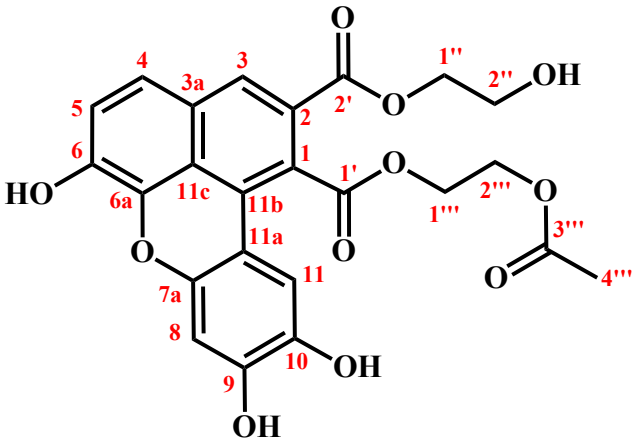


Figure 15S: HMBC spectrum (CD_3COCD_3, 500 MHz) of **30**



31

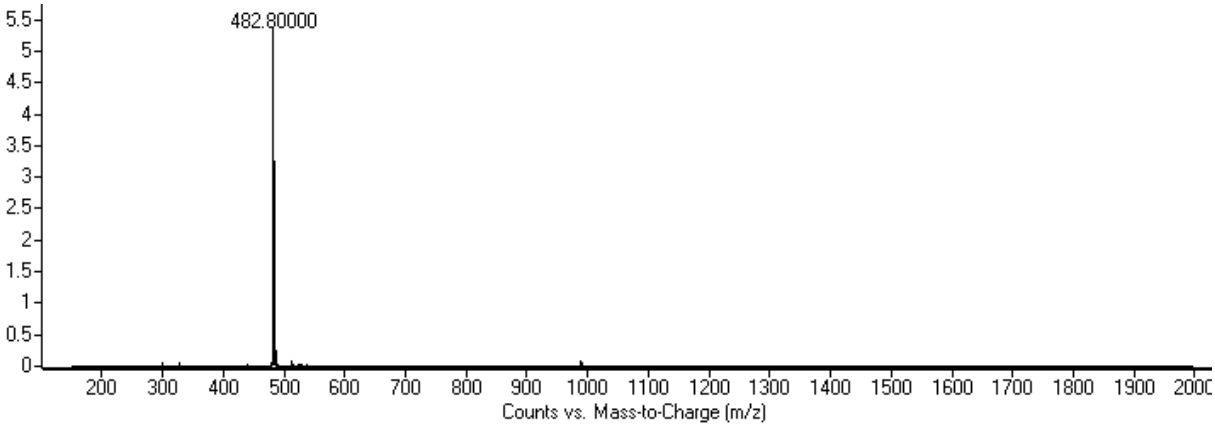


Figure 16S: ESI-MS spectrum of **31**

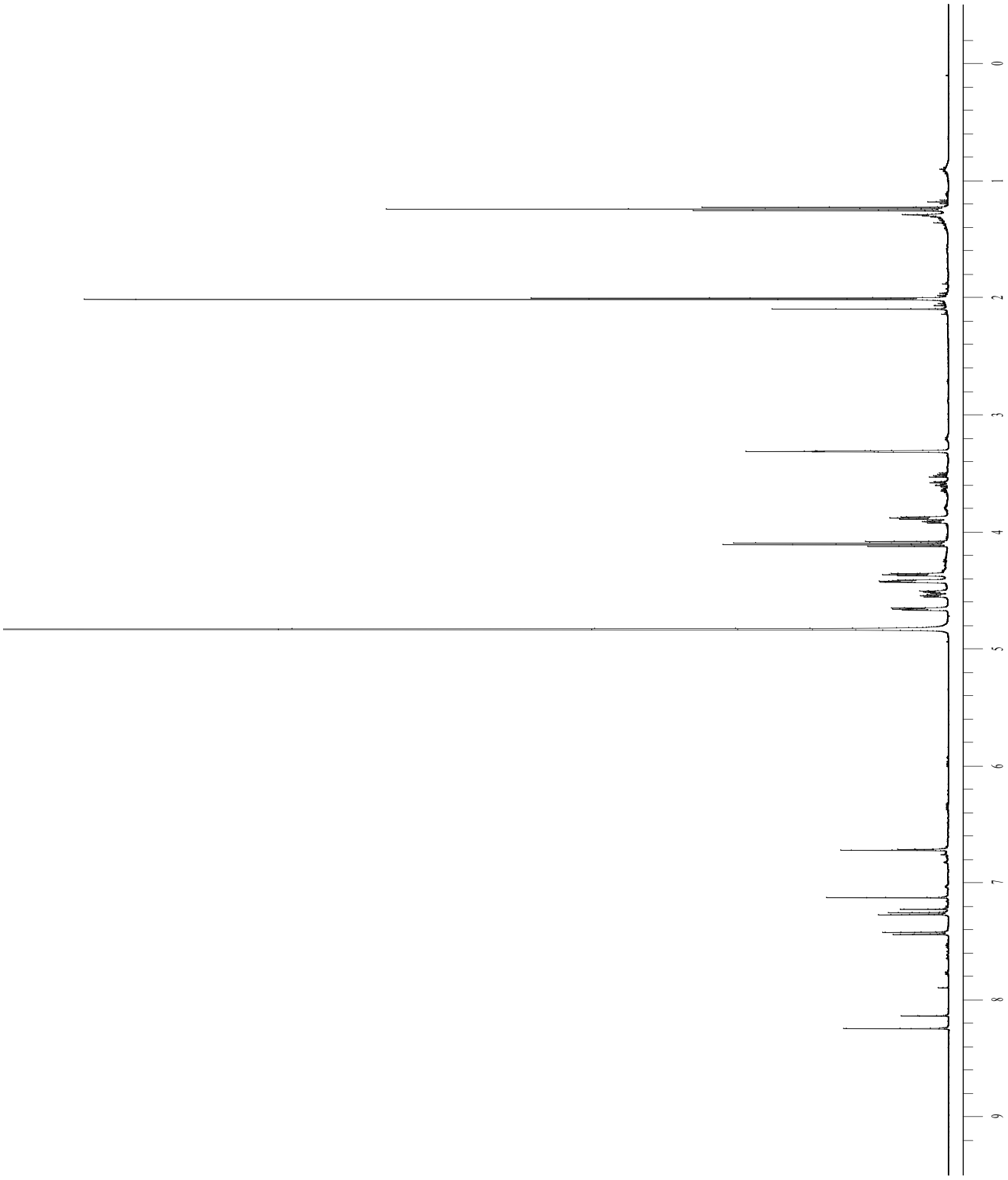


Figure 17S: ^{1}H-NMR spectrum (CD_3COCD_3, 500 MHz) of **31**

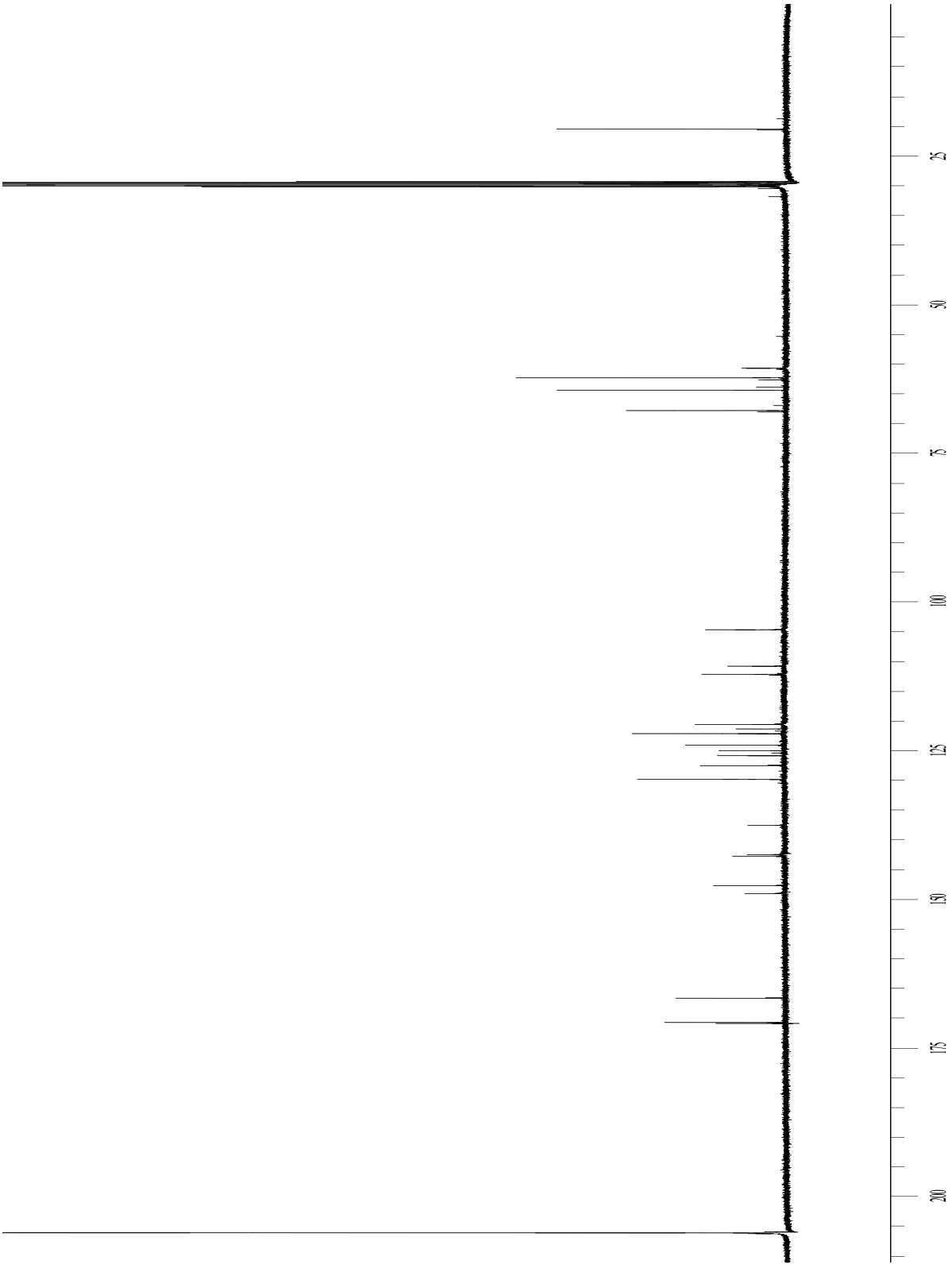


Figure 18S: ^{13}C- NMR spectrum (CD_3COCD_3, 125 MHz) of **31**

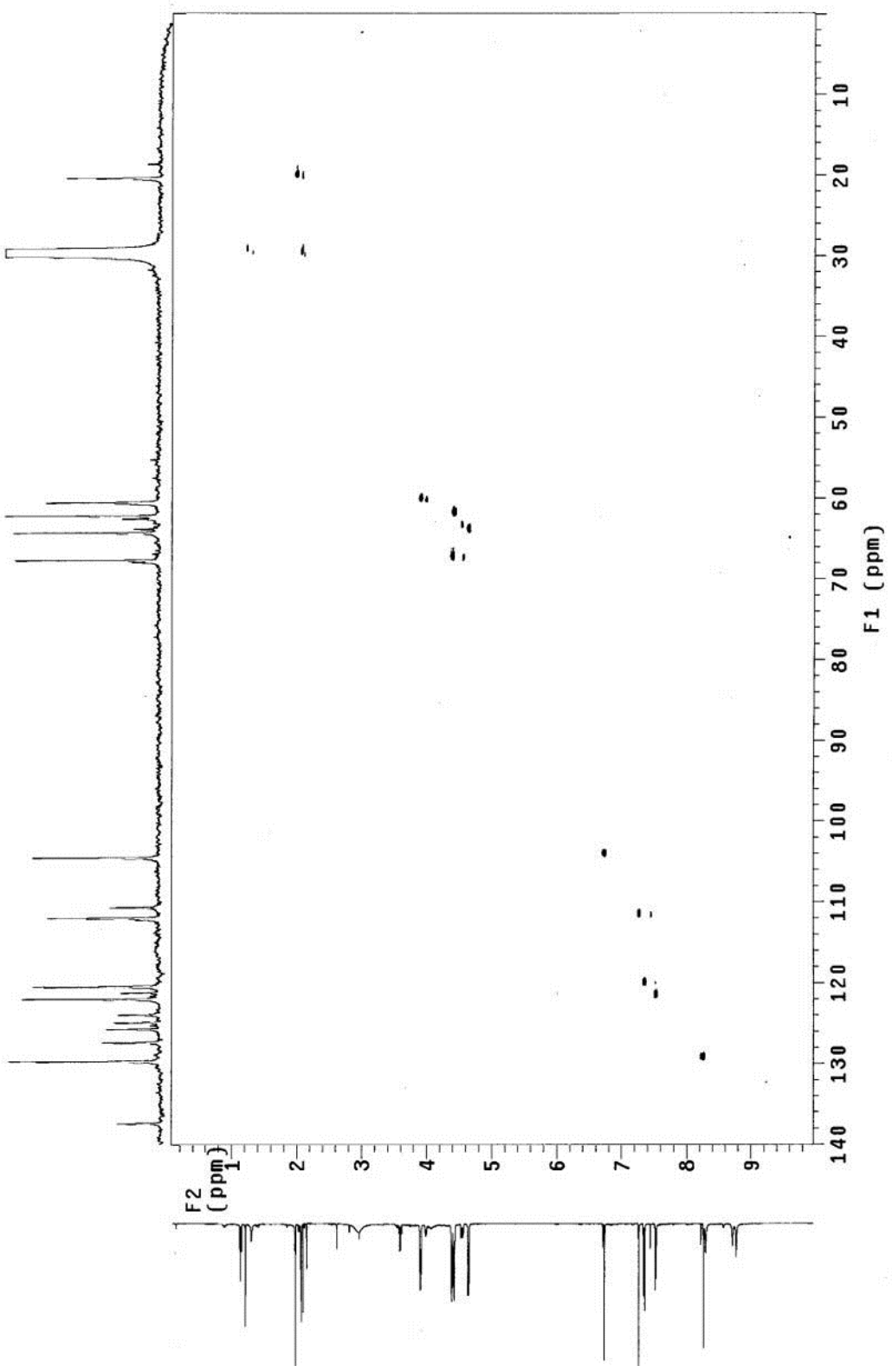


Figure 19S: HSQC spectrum (CD_3COCD_3, 500 MHz) of **31**

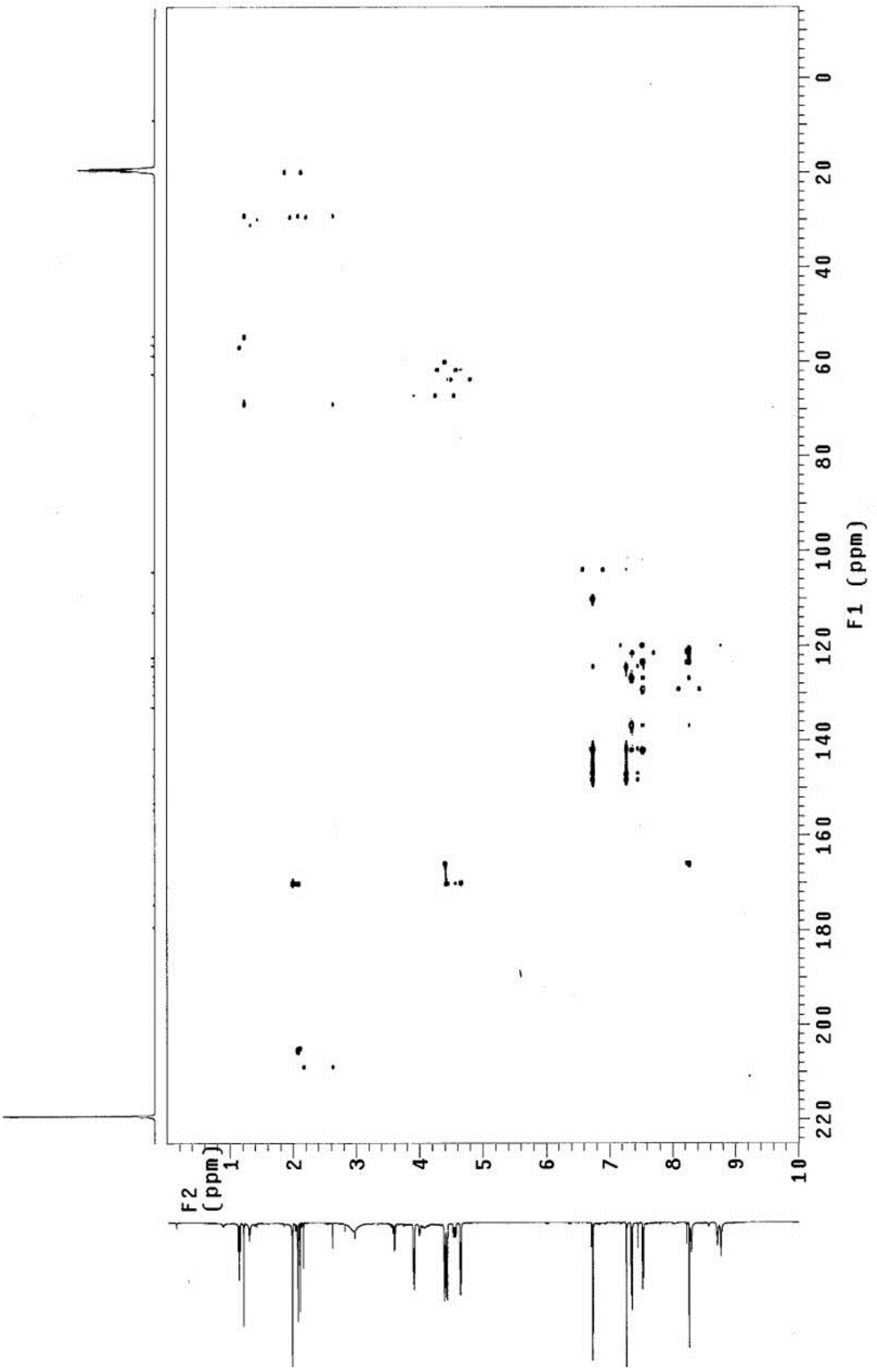
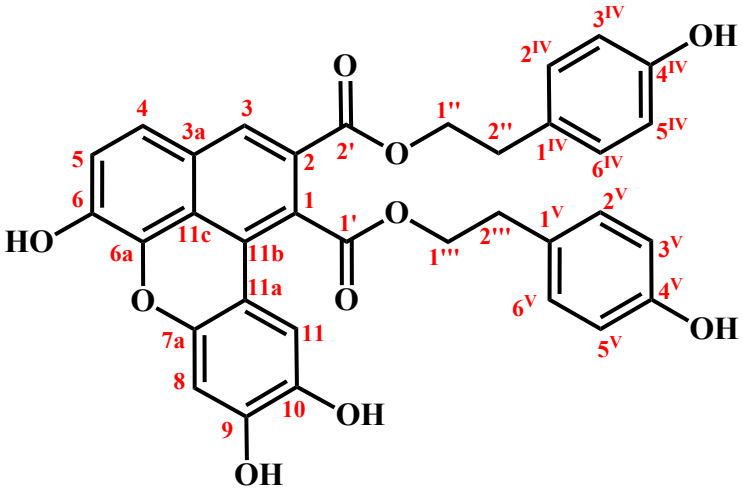


Figure 20S: HMBC spectrum (CD_3COCD_3, 500 MHz) of **31**



32

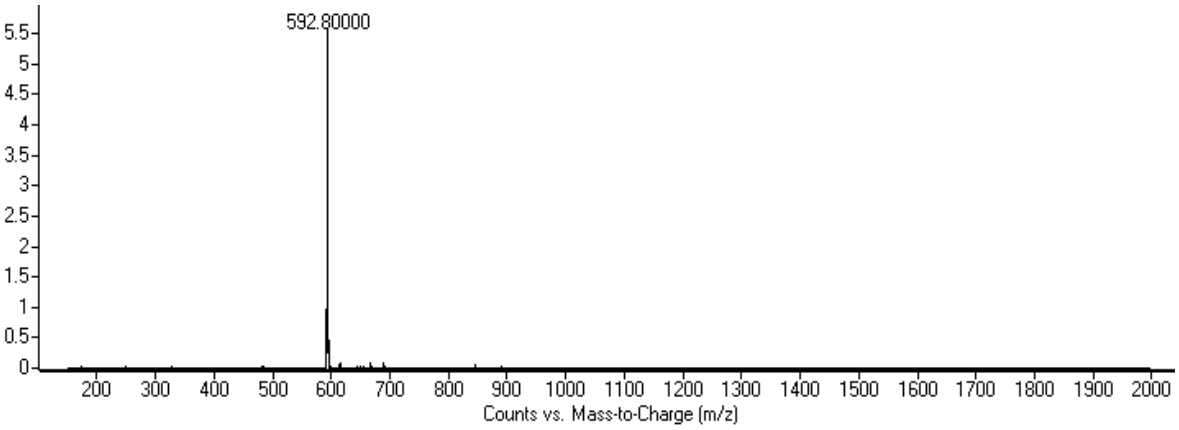


Figure 21S: ESI-MS spectrum of **32**

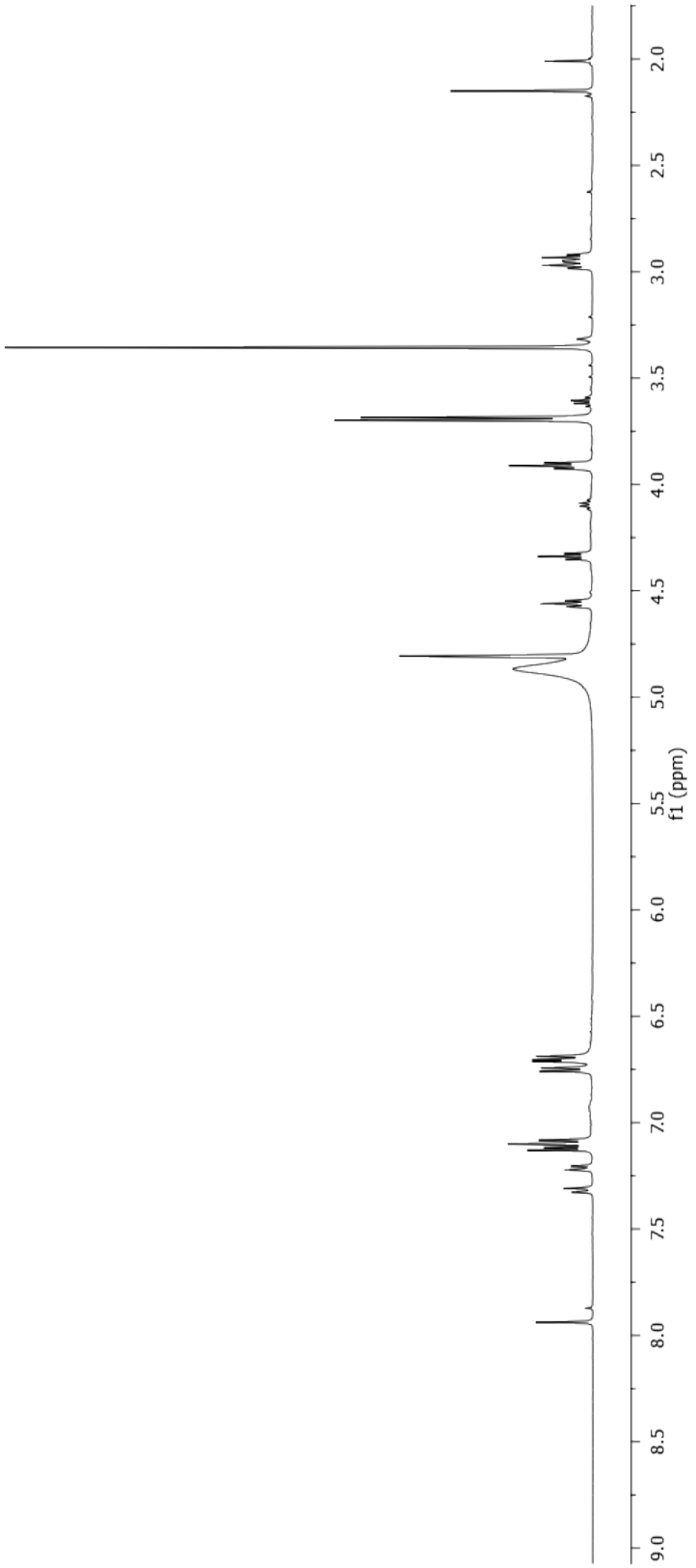


Figure 22S: ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of **32**

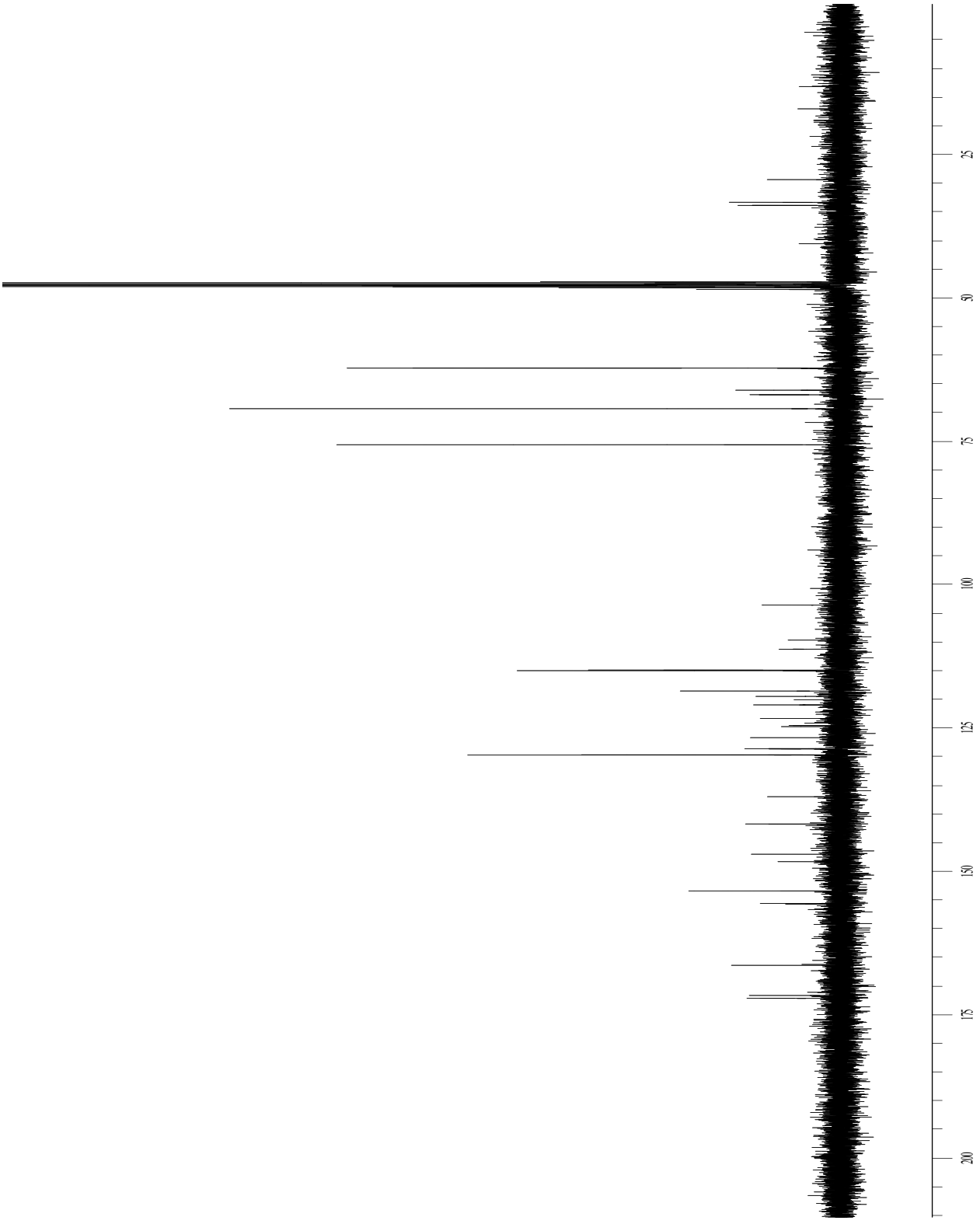


Figure 23S: ^{13}C- NMR spectrum (CD_3OD, 125 MHz) of **32**

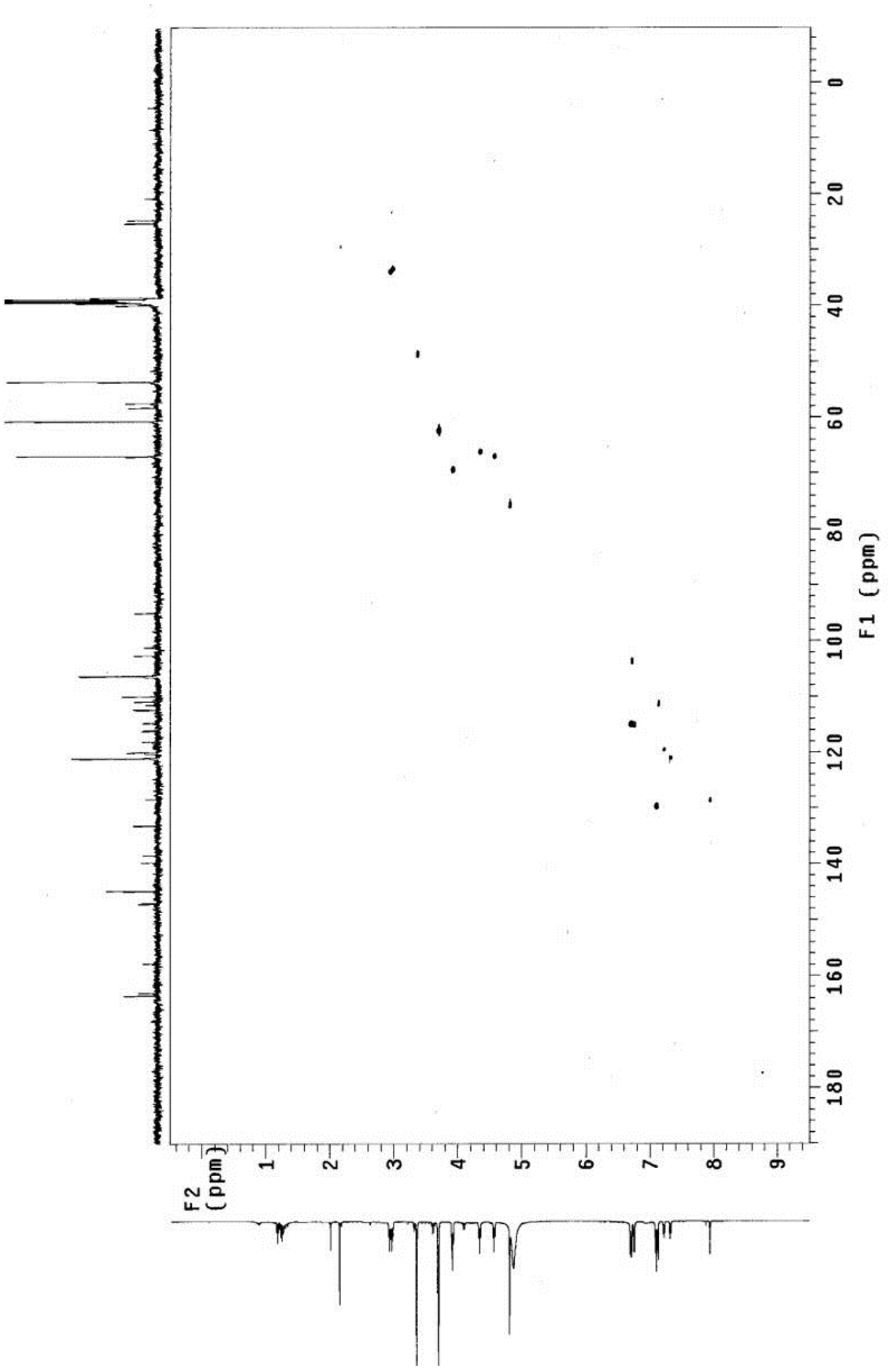


Figure 24S: HSQC spectrum (CD_3OD, 500 MHz) of **32**

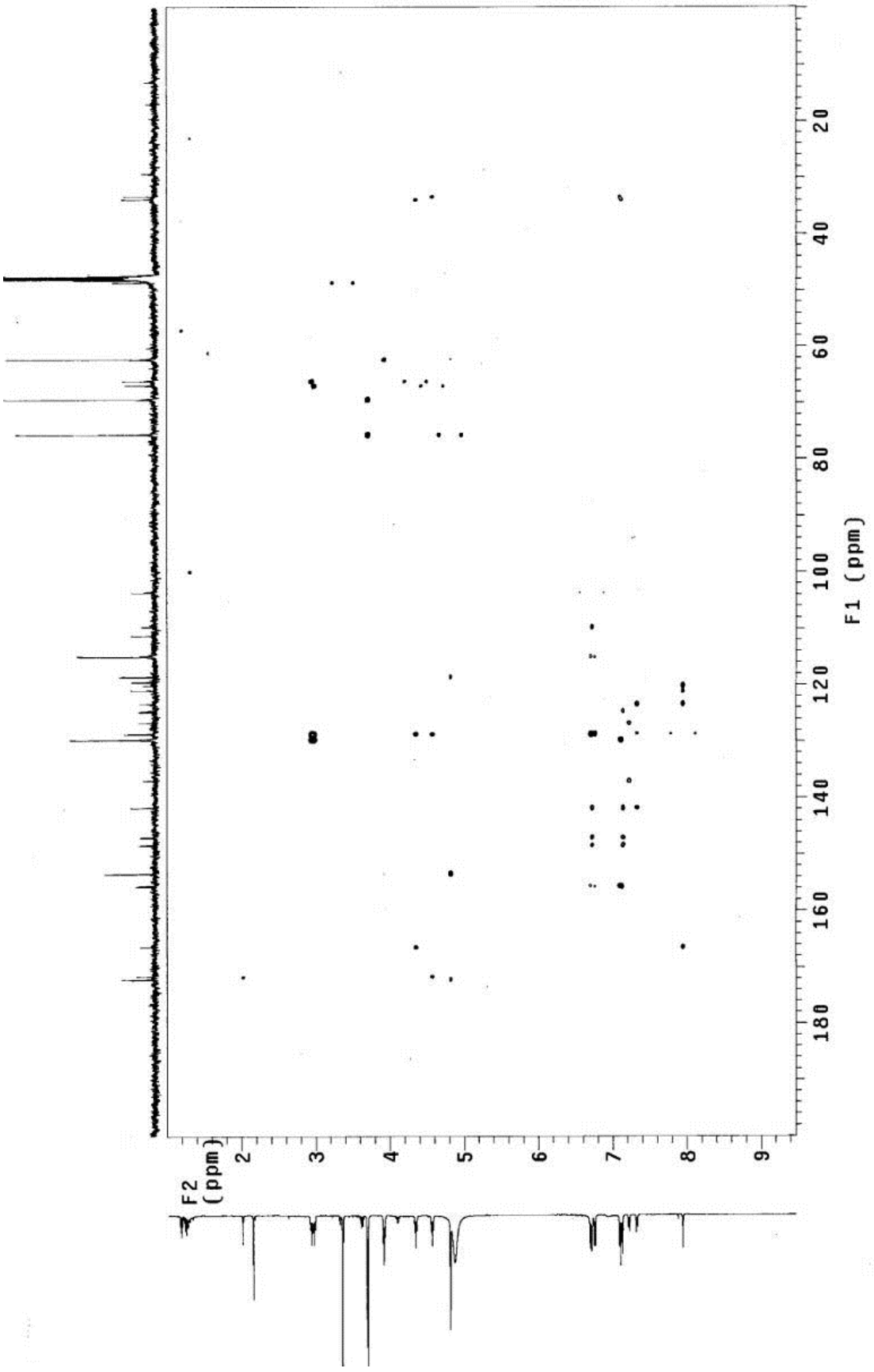
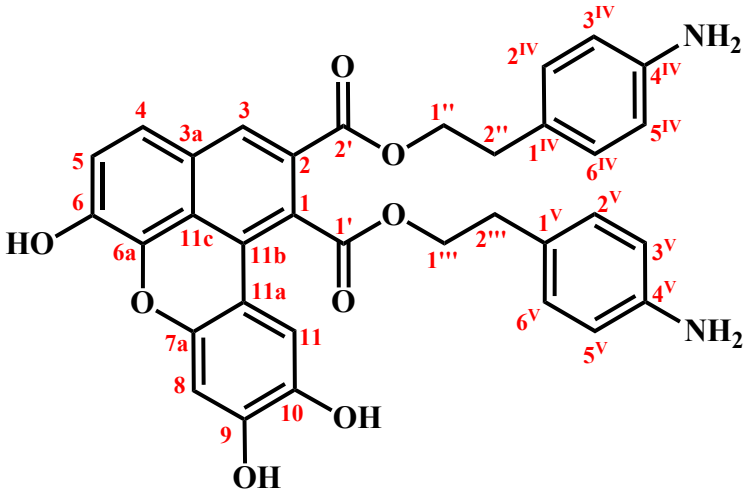


Figure 25S: HMBC spectrum (CD_3OD, 500 MHz) of **32**



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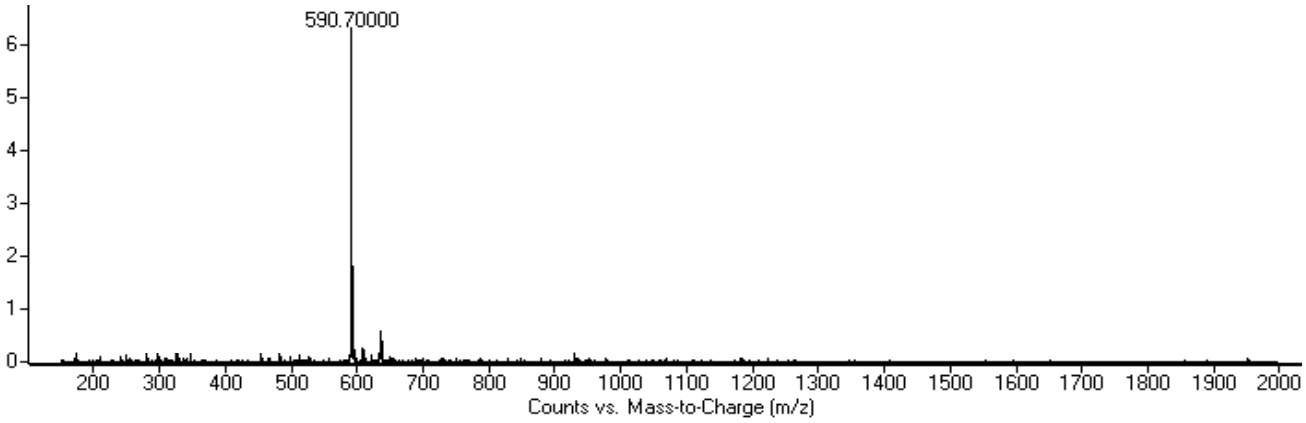


Figure 26S: ESI-MS spectrum of **33**

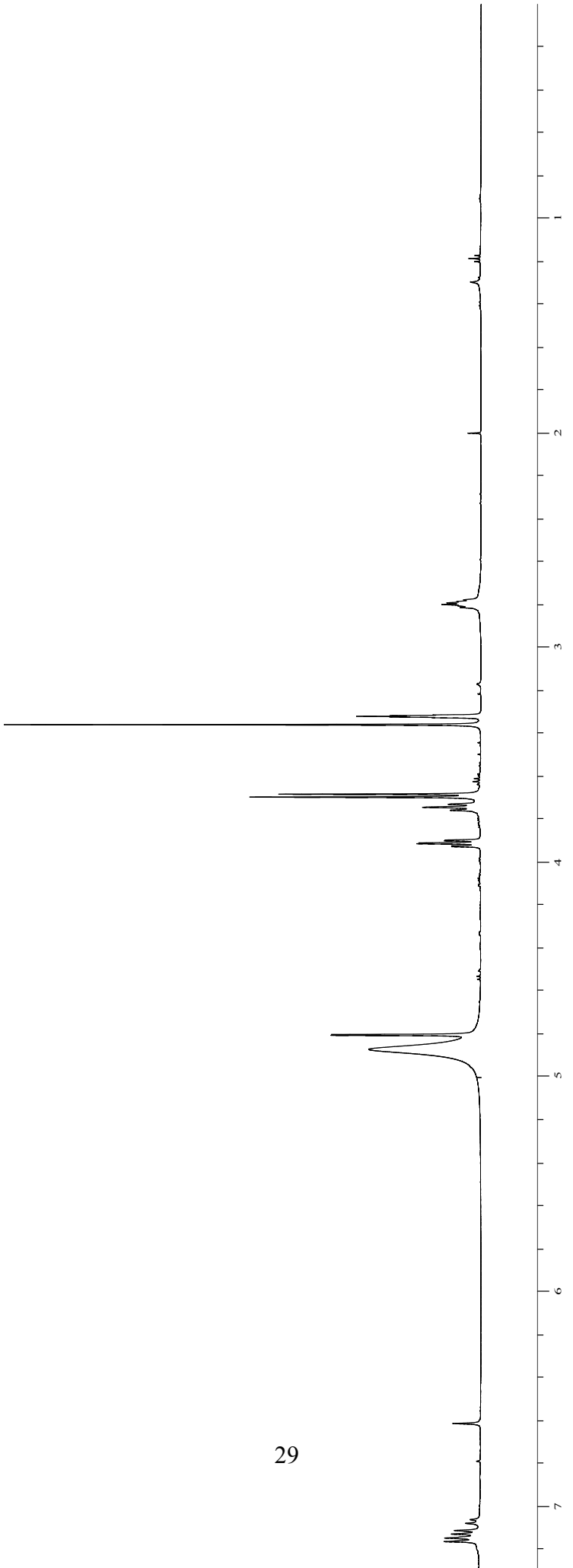


Figure 27S: ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of **33**

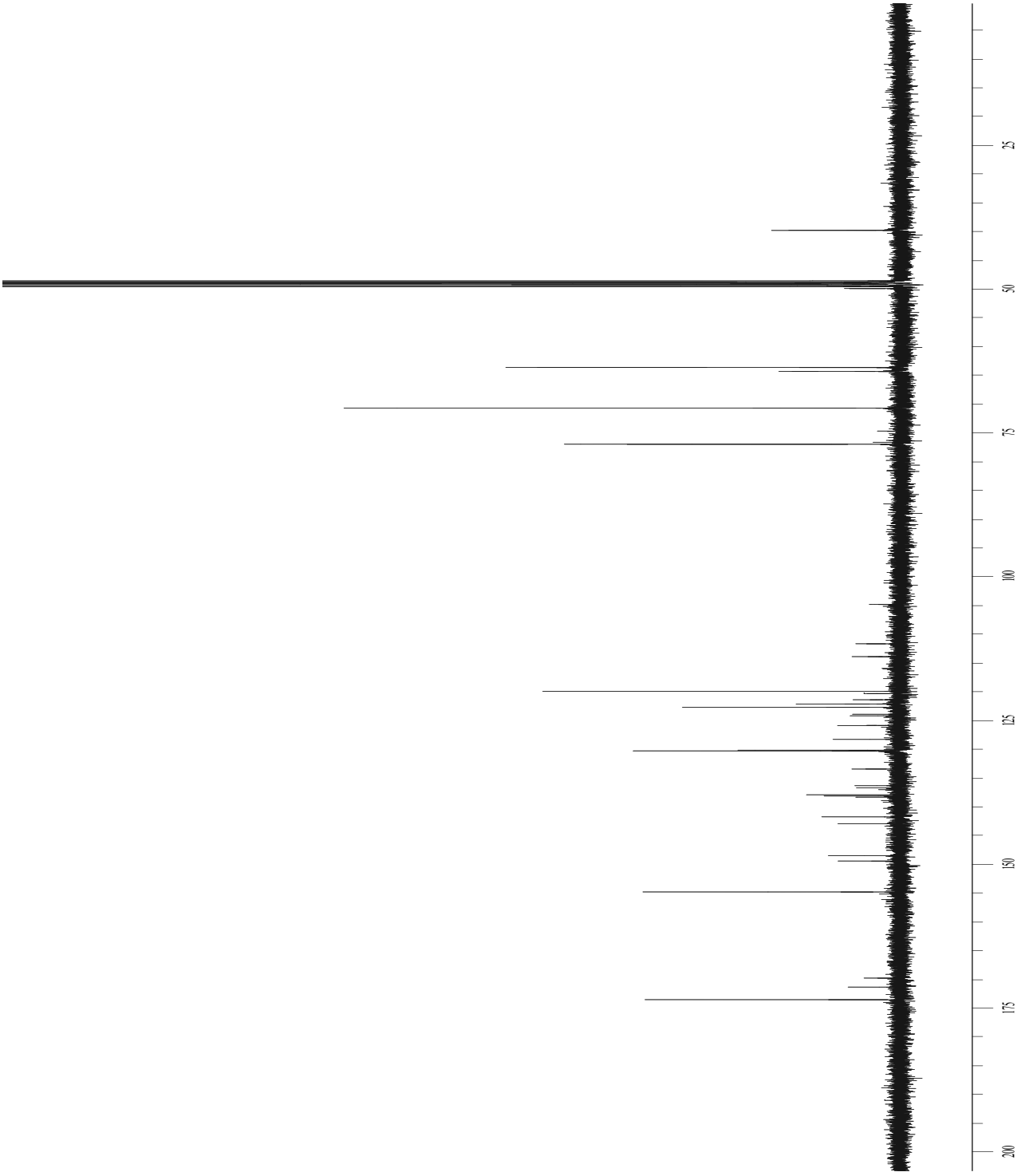


Figure 28S: ^{13}C- NMR spectrum (CD_3OD, 125 MHz) of **33**

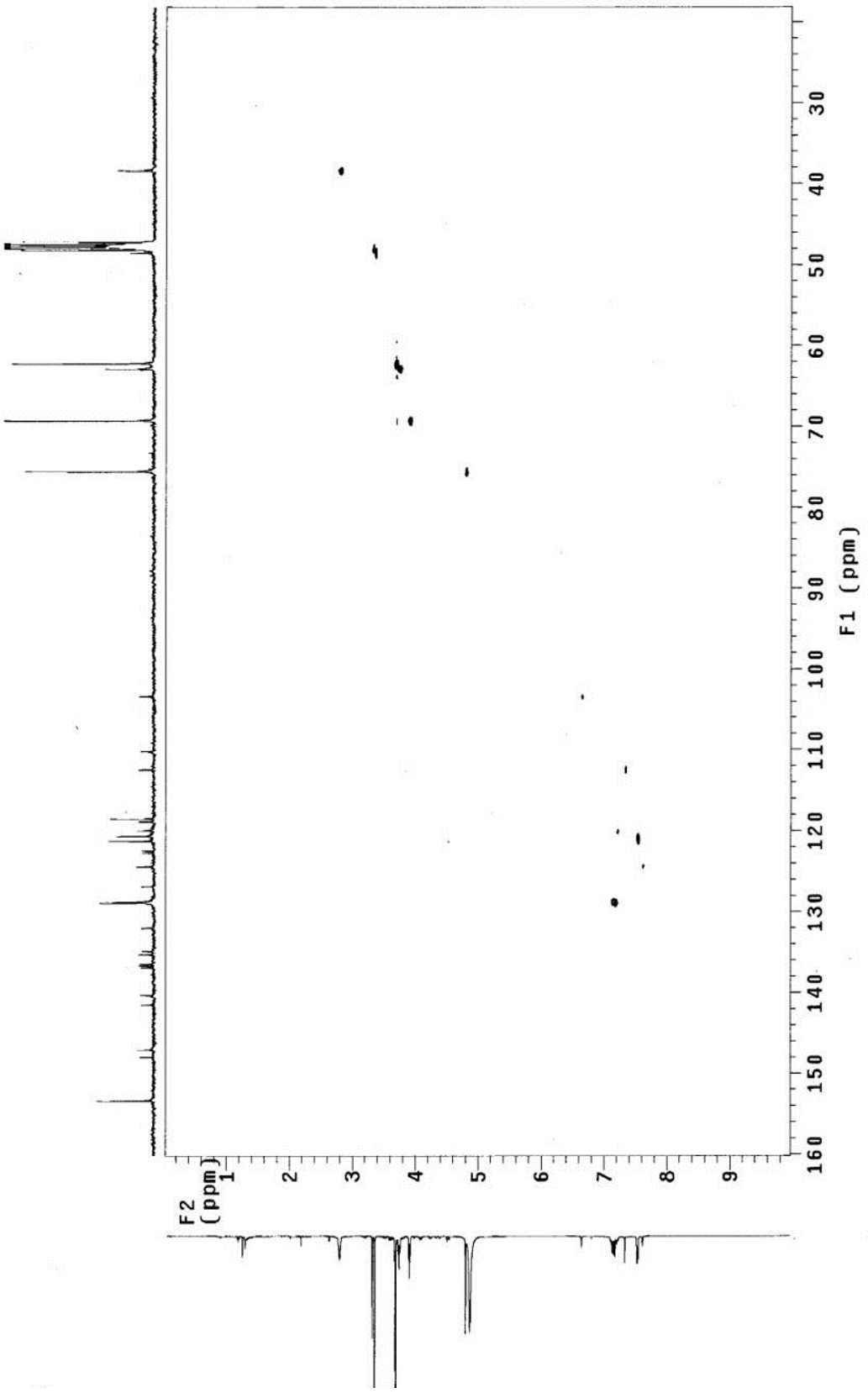


Figure 29S: HSQC spectrum (CD_3OD, 500 MHz) of **33**

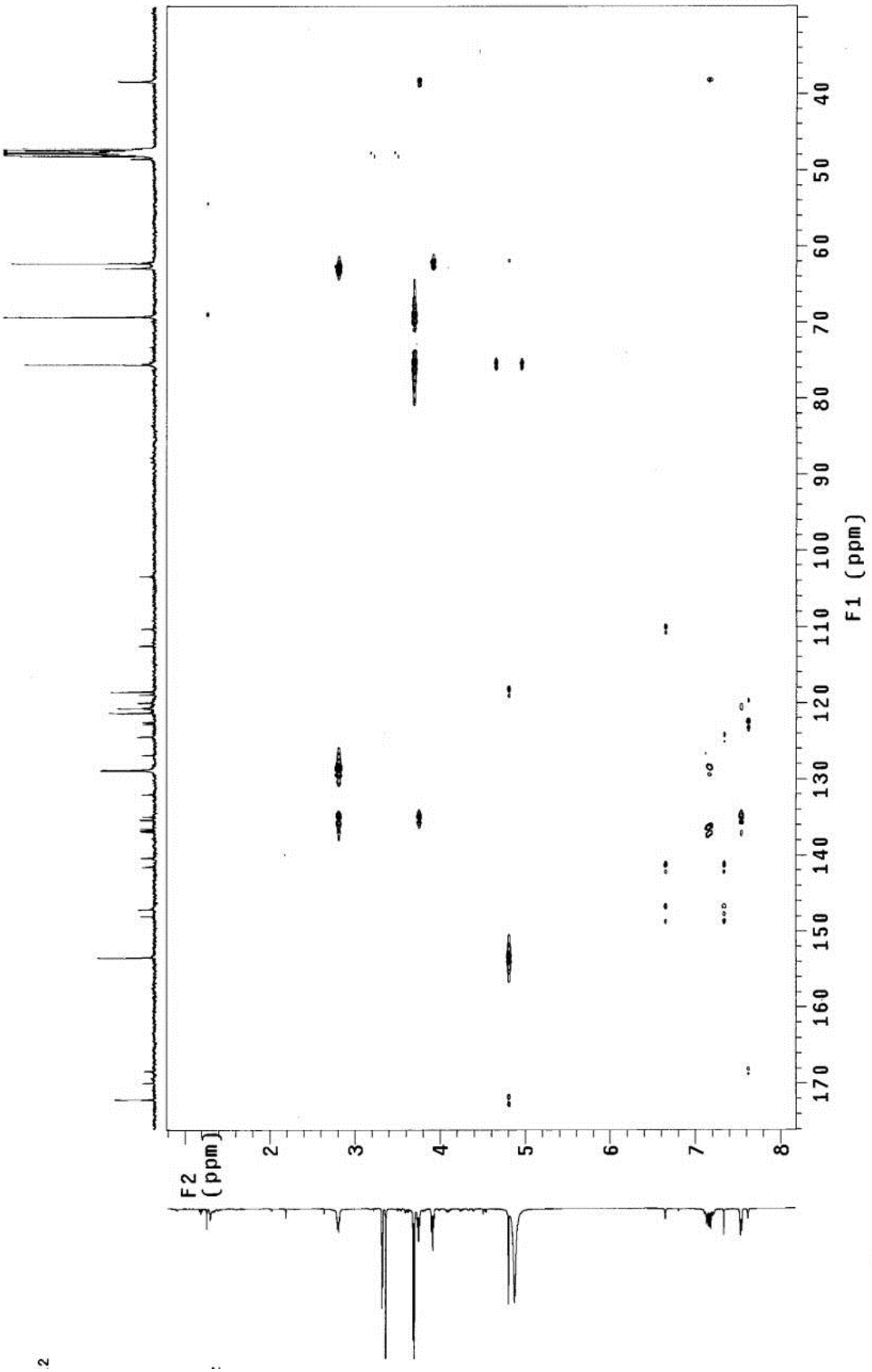
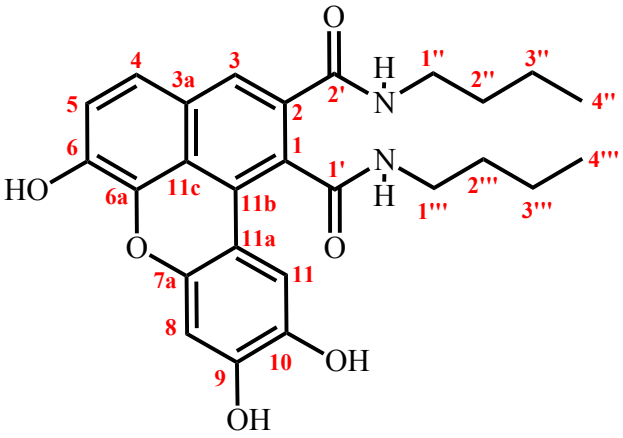


Figure 30S: HMBC spectrum (CD_3OD, 500 MHz) of **33**



34

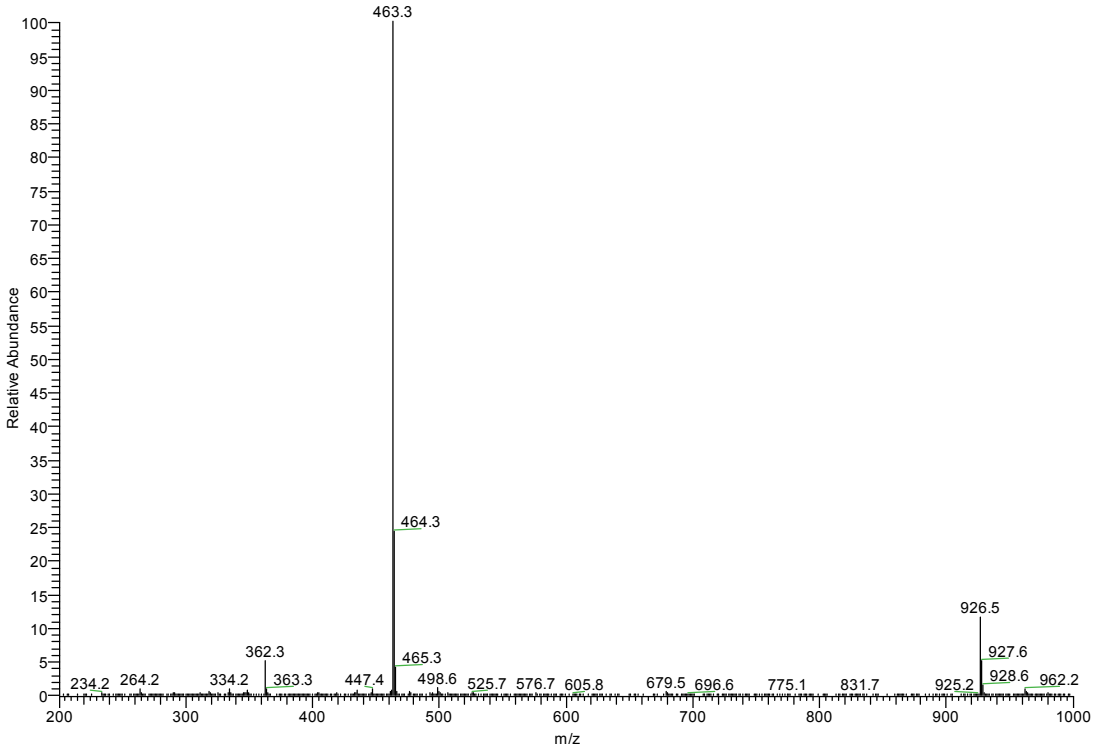


Figure 31S: ESI-MS spectrum of **34**

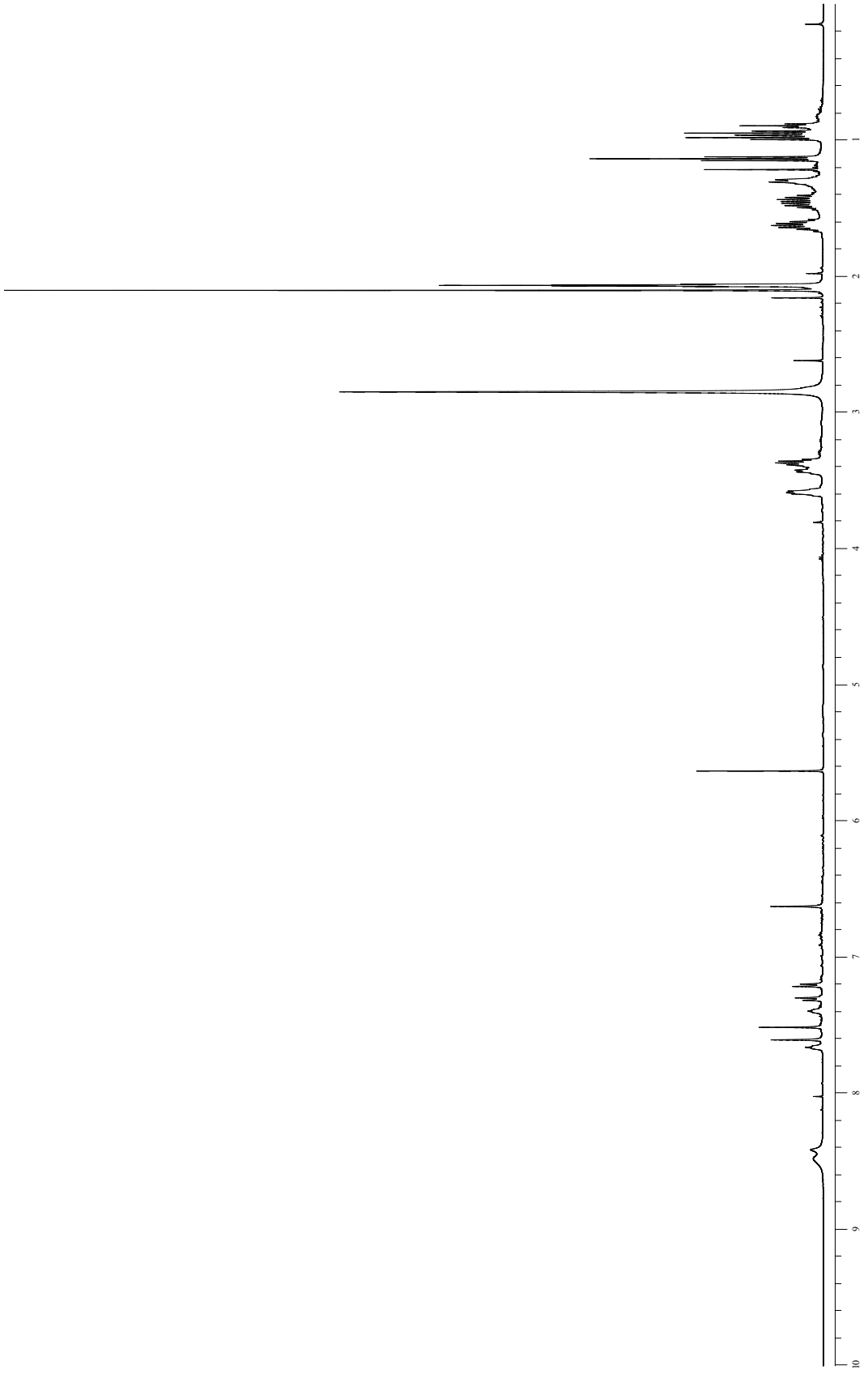


Figure 32S: ^{1}H-NMR spectrum (CD_3COCD_3, 500 MHz) of **34**

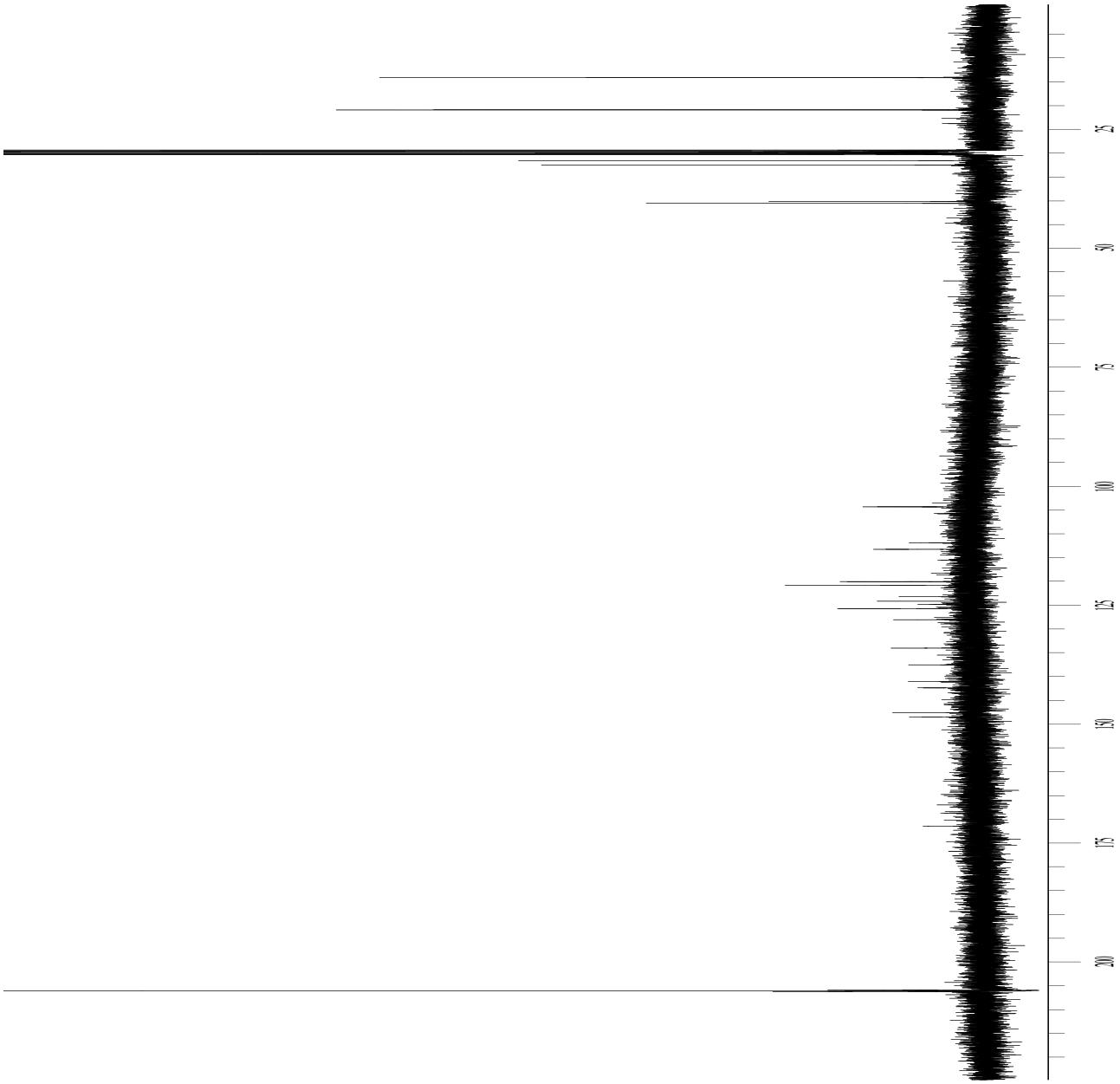


Figure 33S: ^{13}C- NMR spectrum (CD_3COCD_3, 125 MHz) of **34**

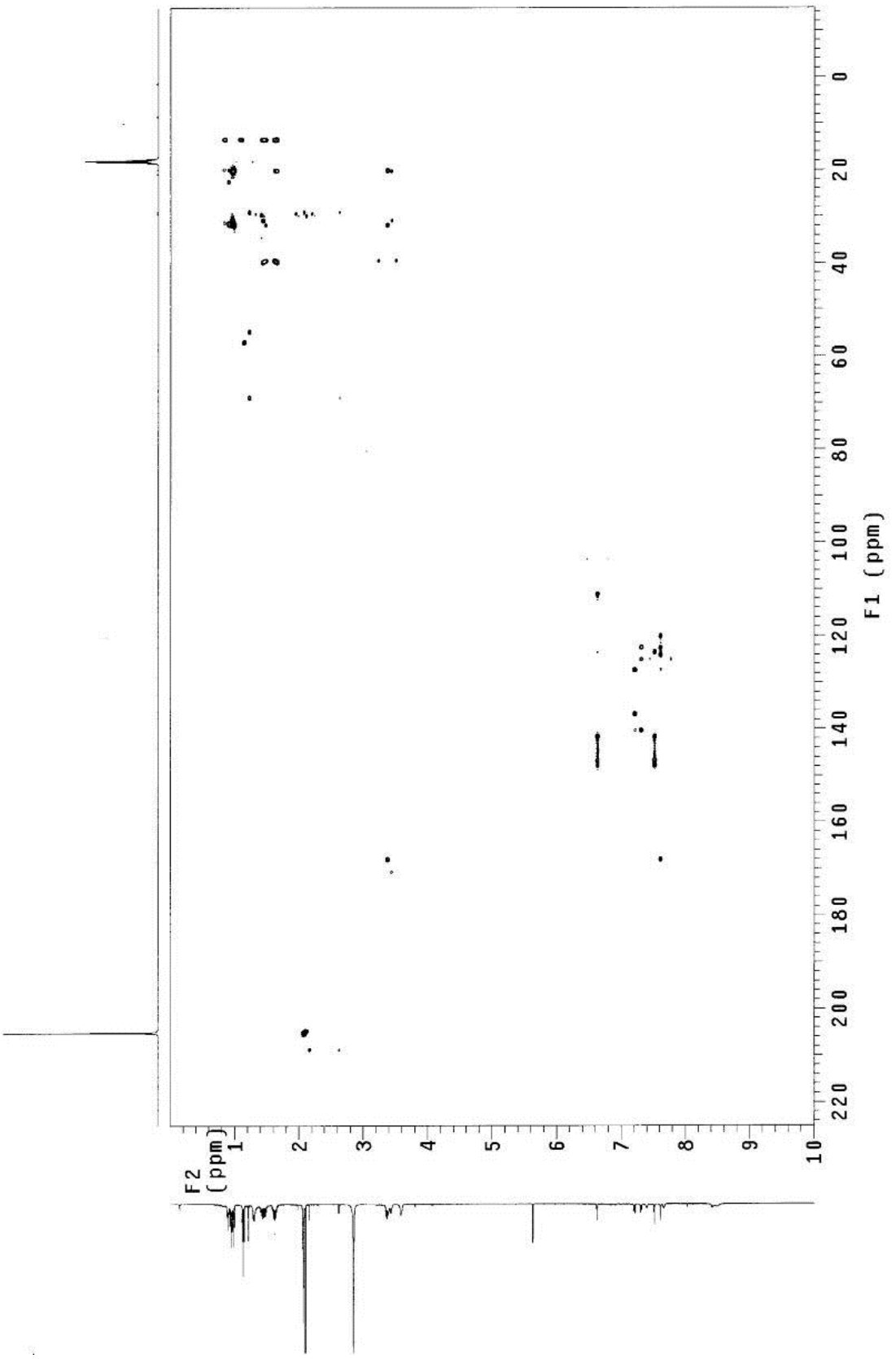
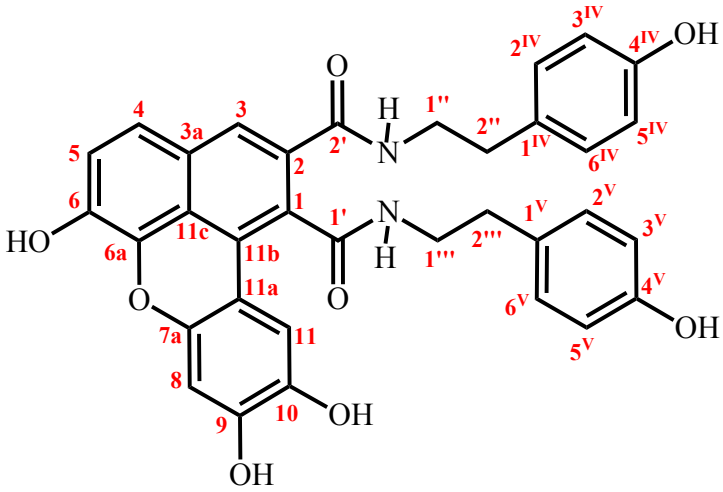


Figure 34S: HMBC spectrum (CD_3COCD_3, 500 MHz) of **34**



35

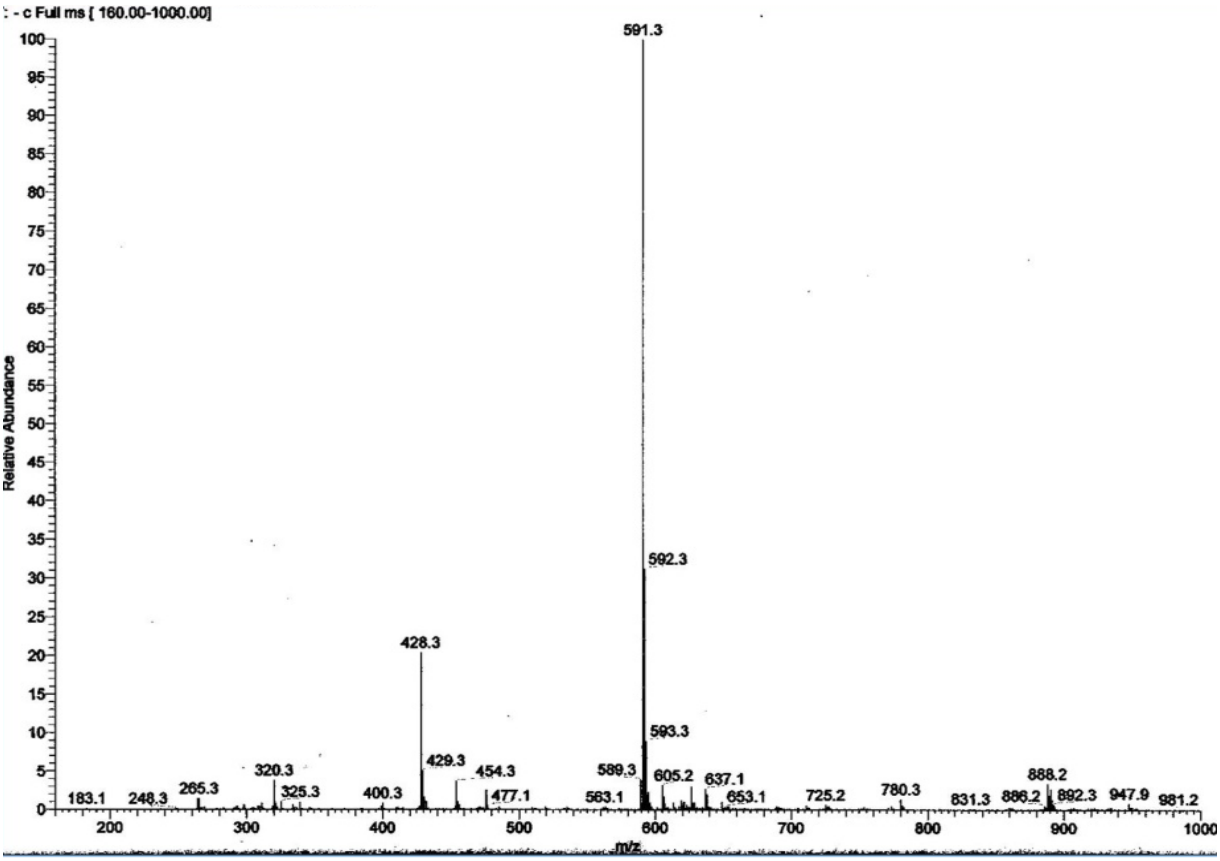


Figure 35S: ESI-MS spectrum of **35**

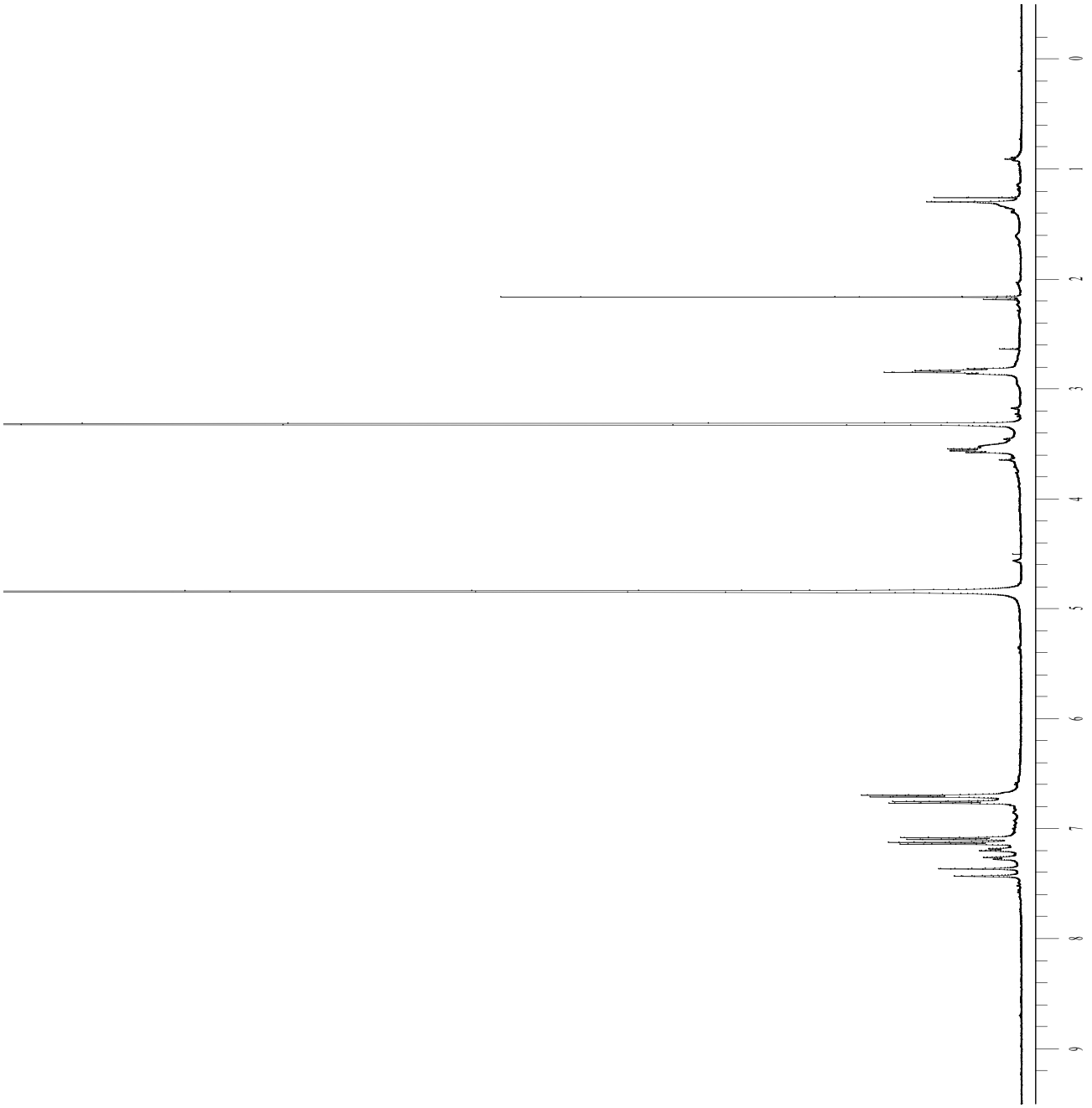


Figure 36S: ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of **35**

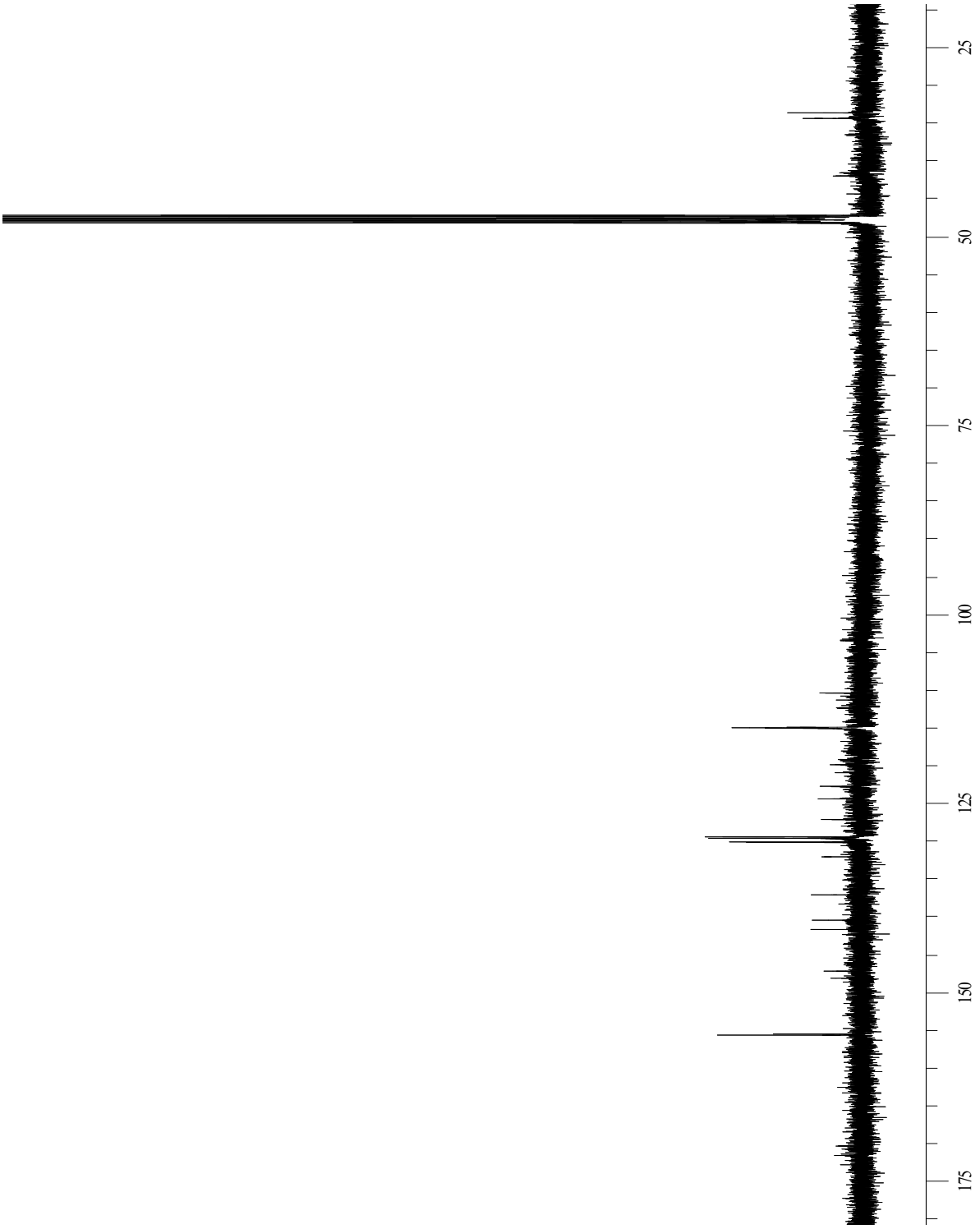


Figure 37S: ^{13}C- NMR spectrum (CD_3OD, 125 MHz) of **35**

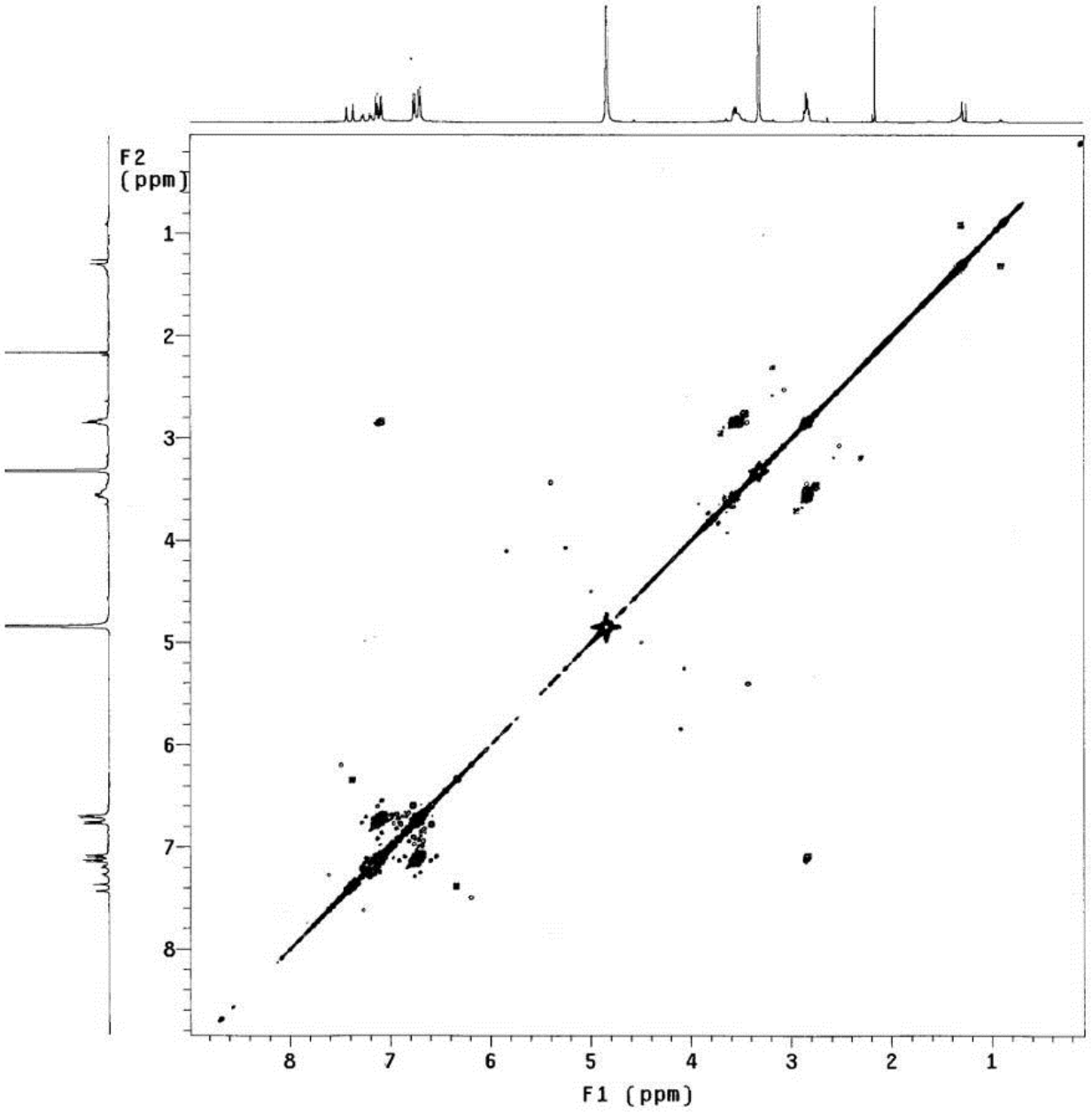
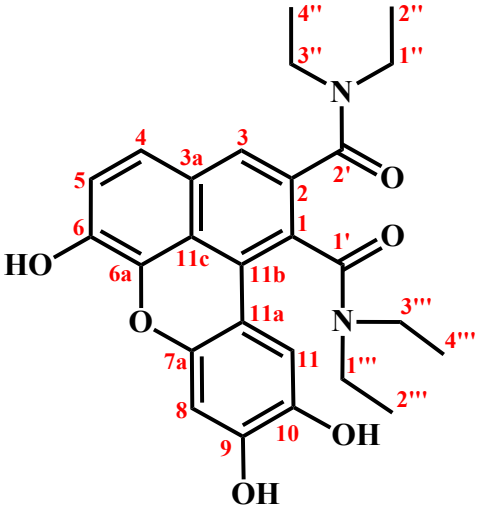


Figure 38S: COSY spectrum (CD_3OD, 500 MHz) of **35**



36

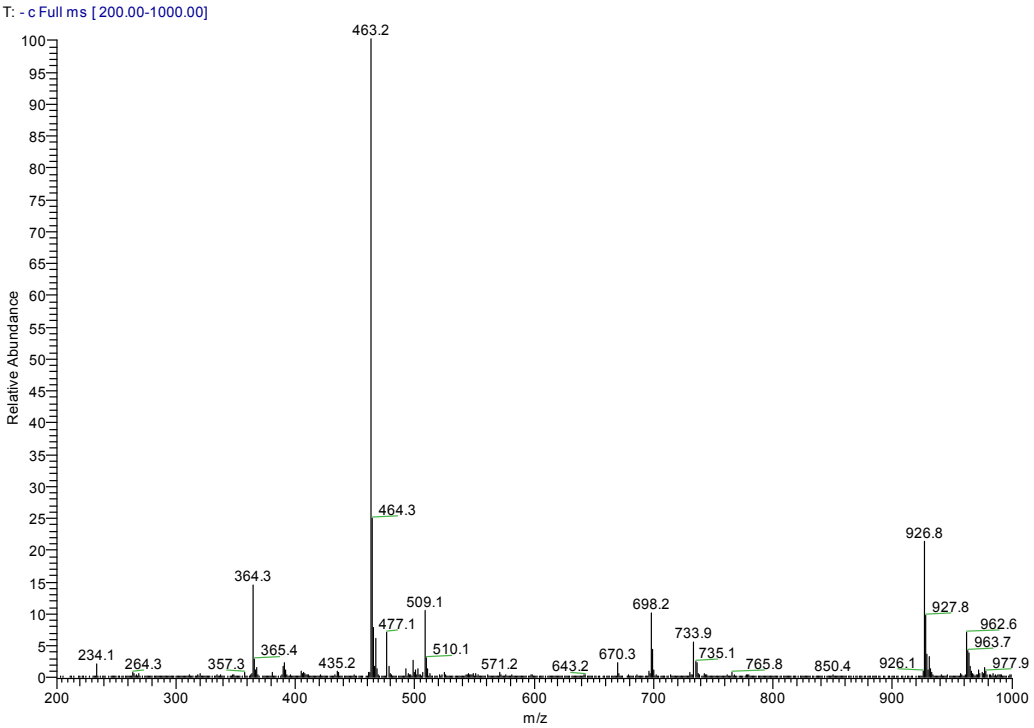


Figure 39S: ESI-MS spectrum of **36**

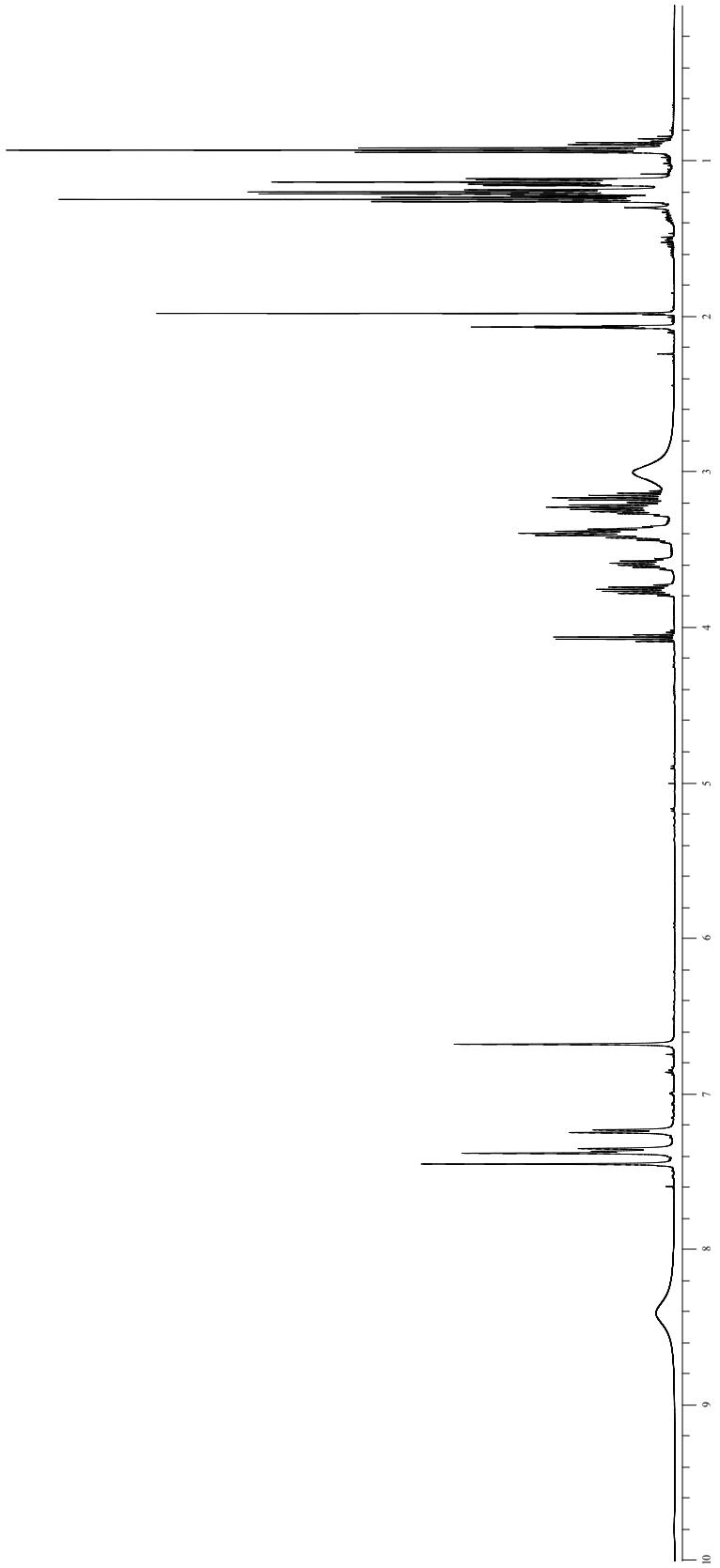


Figure 40S: ^{1}H-NMR spectrum (CD_3COCD_3, 500 MHz) of **36**

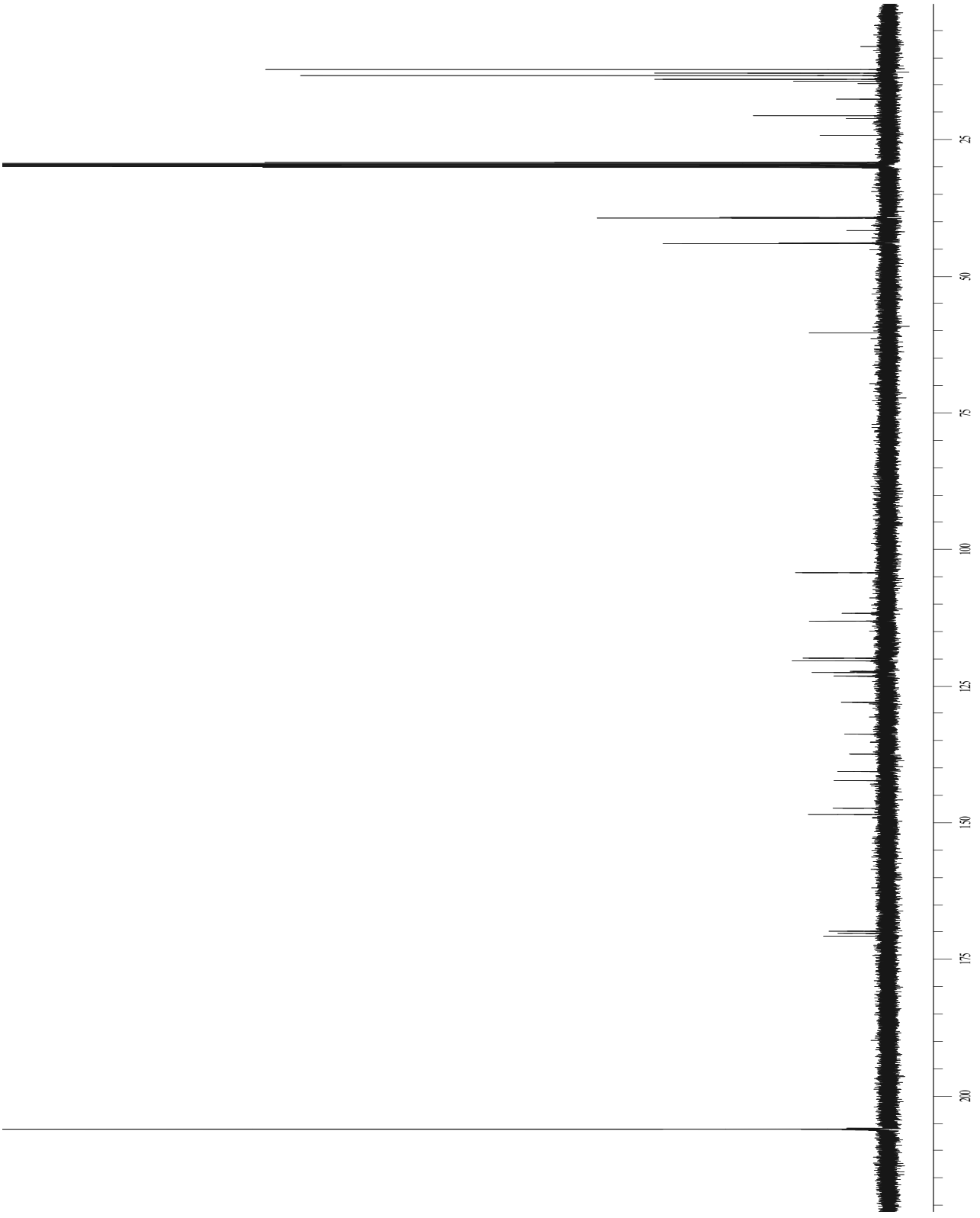


Figure 41S: ^{13}C- NMR spectrum (CD_3COCD_3, 125 MHz) of **36**

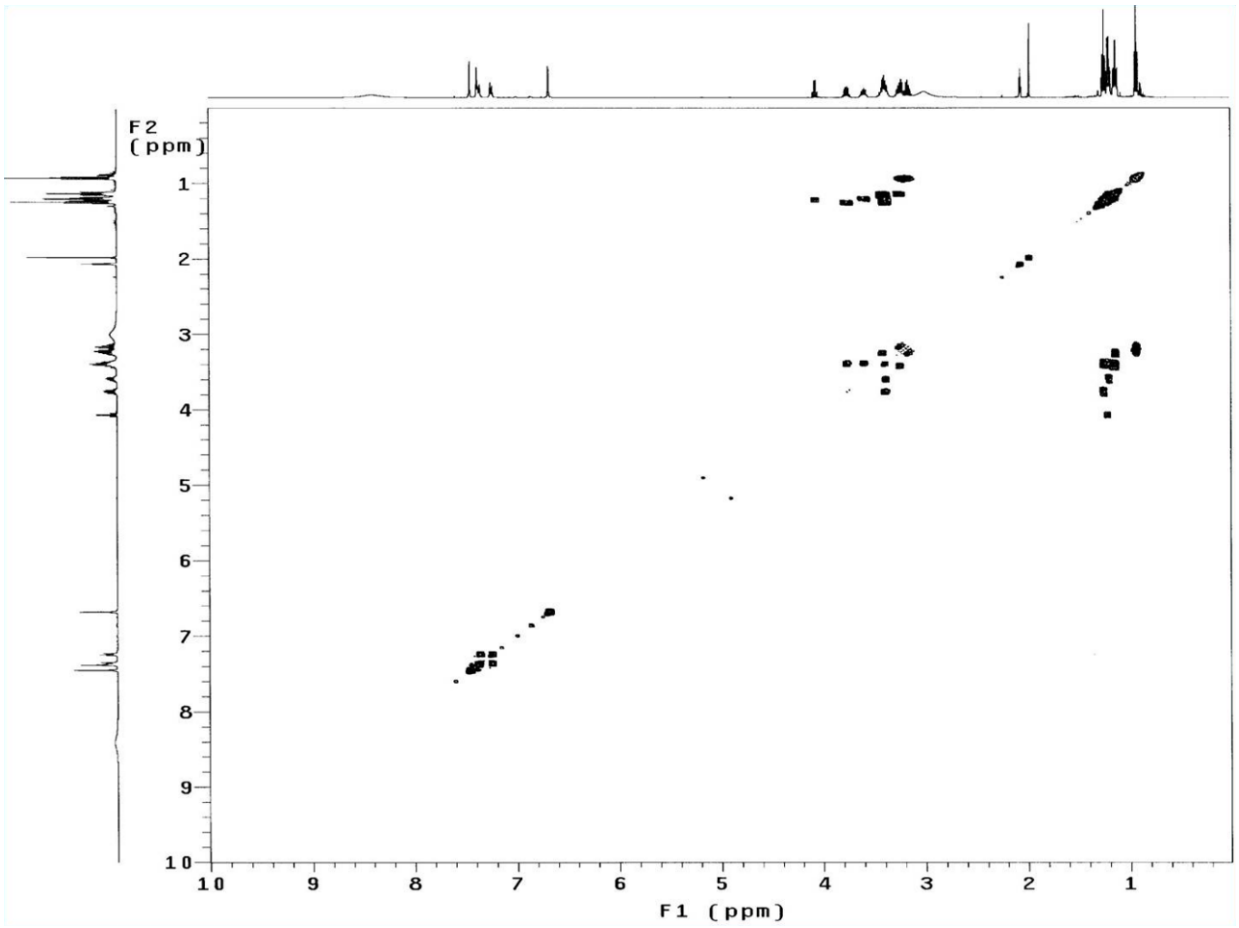


Figure 42S: COSY spectrum (CD_3OD, 500 MHz) of **36**

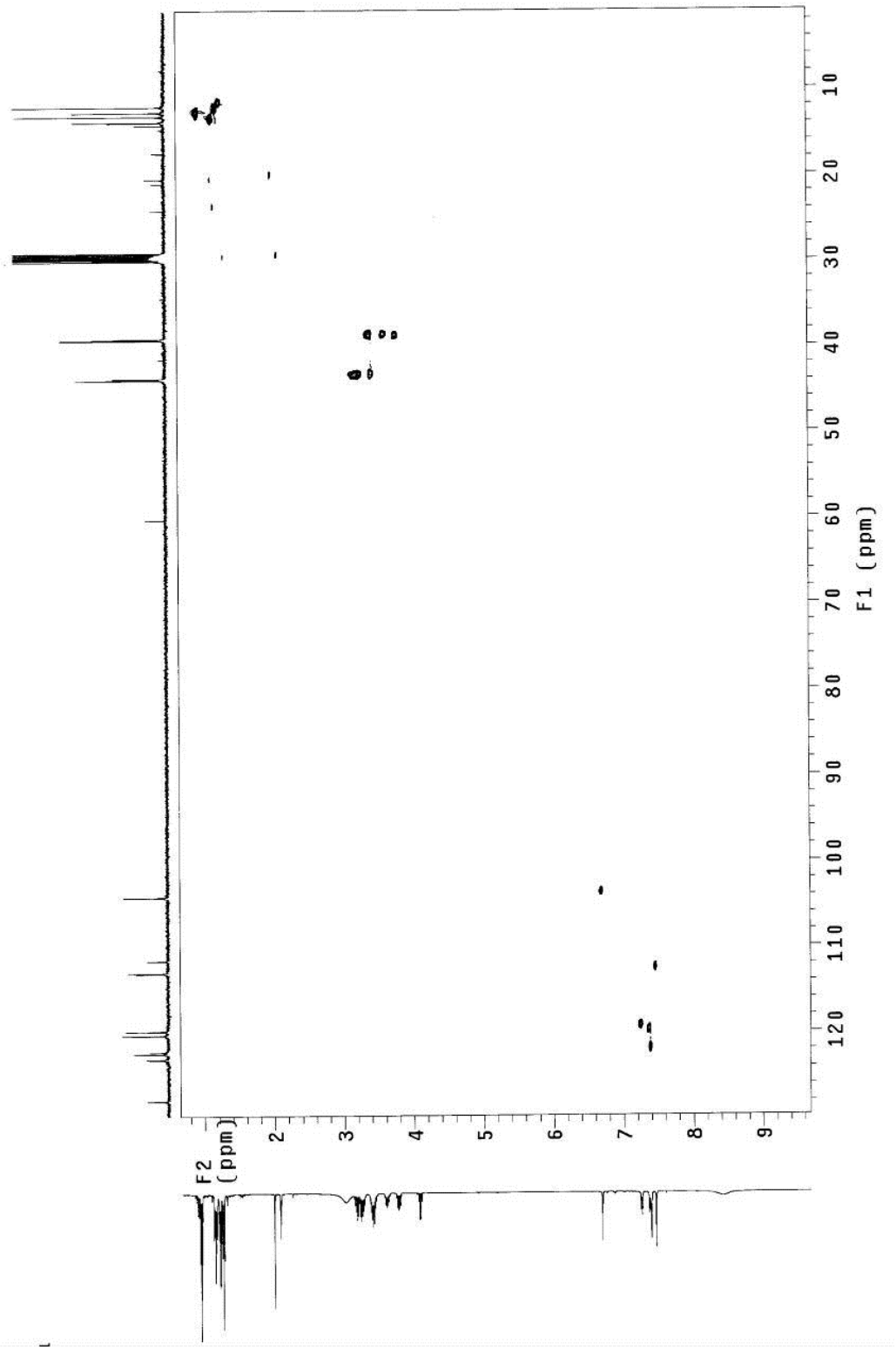


Figure 43S: HSQC spectrum (CD_3OD, 500 MHz) of **36**

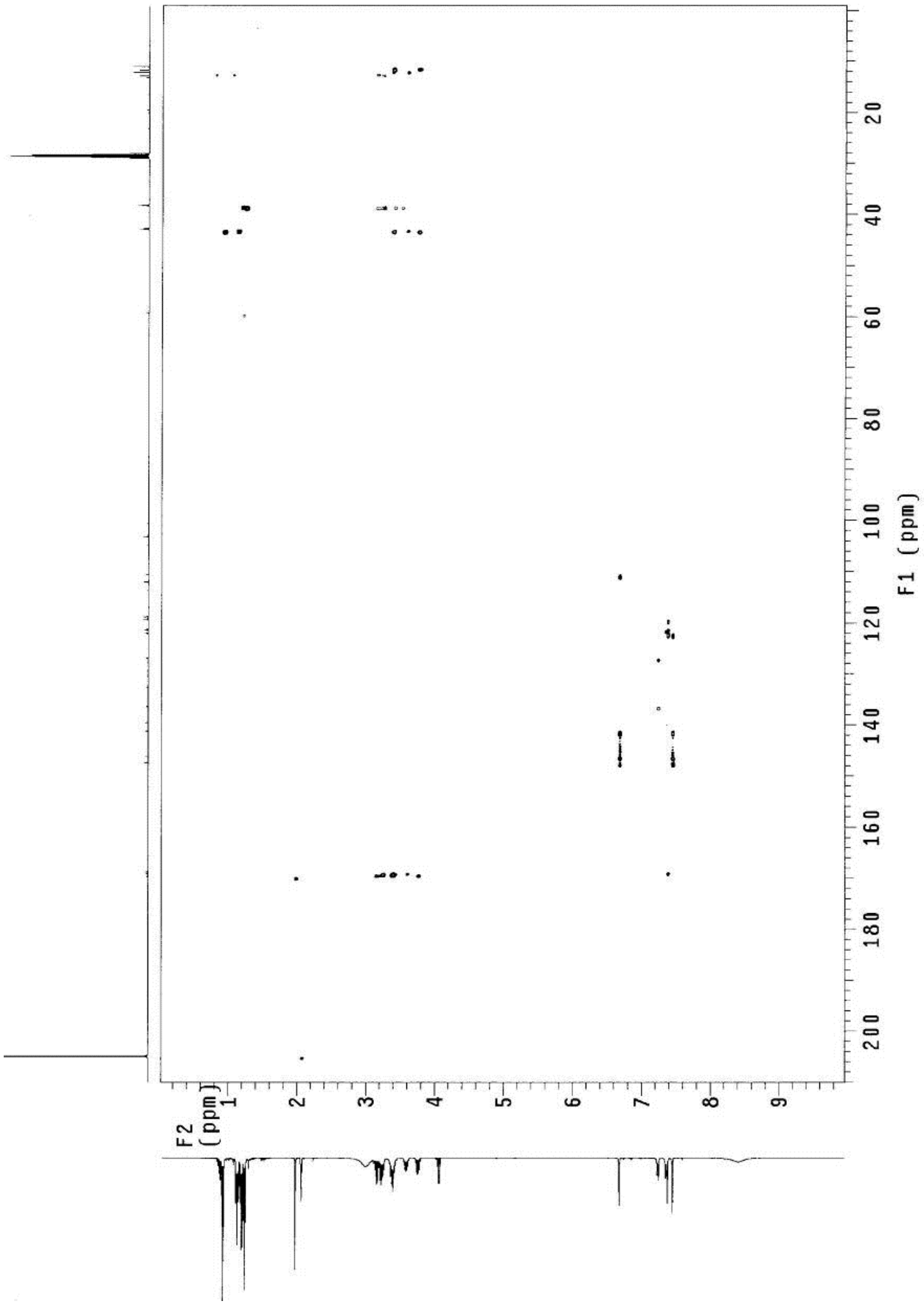


Figure 44S: HMBC spectrum (CD_3COCD_3, 500 MHz) of **36**

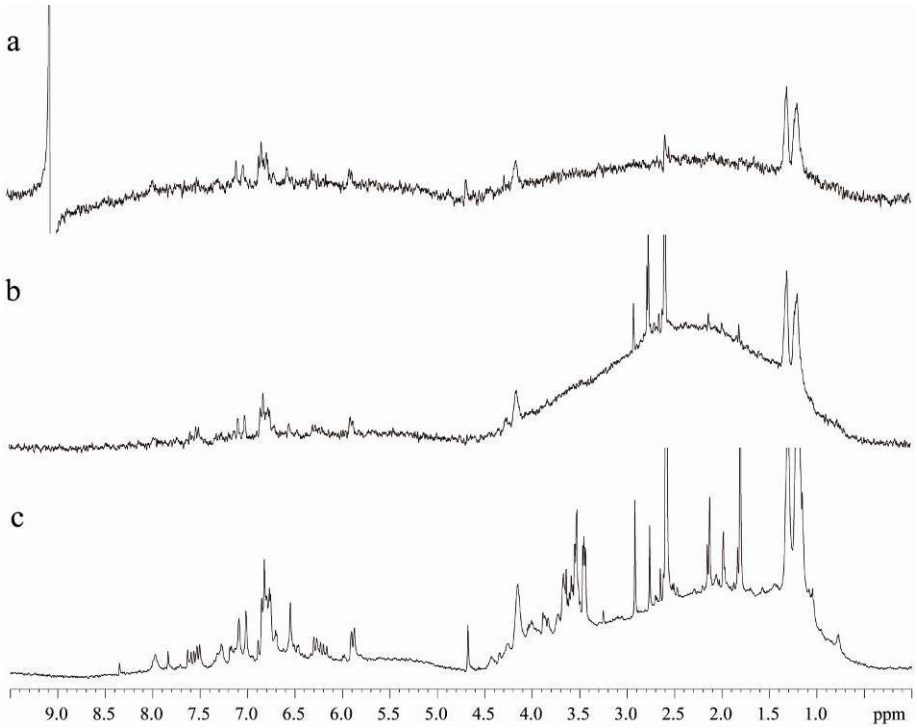


Figure 45S. DF-STD spectra of the **27** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (8.8 ppm) and deoxyribose/backbone (5.4 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

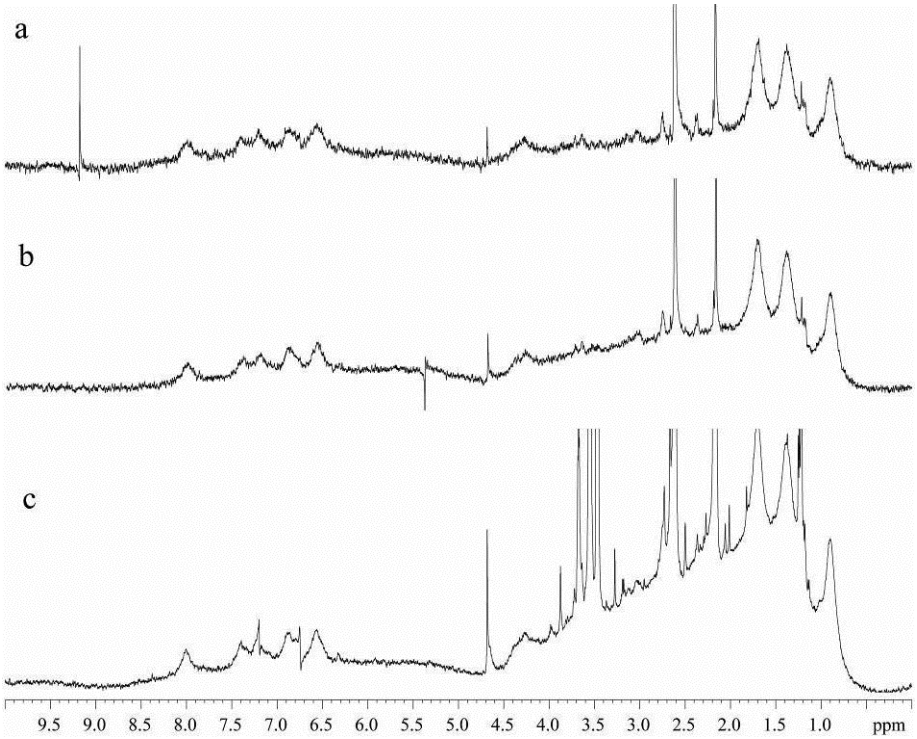


Figure 46S. DF-STD spectra of the **28** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (9.2 ppm) and deoxyribose/backbone (5.4 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

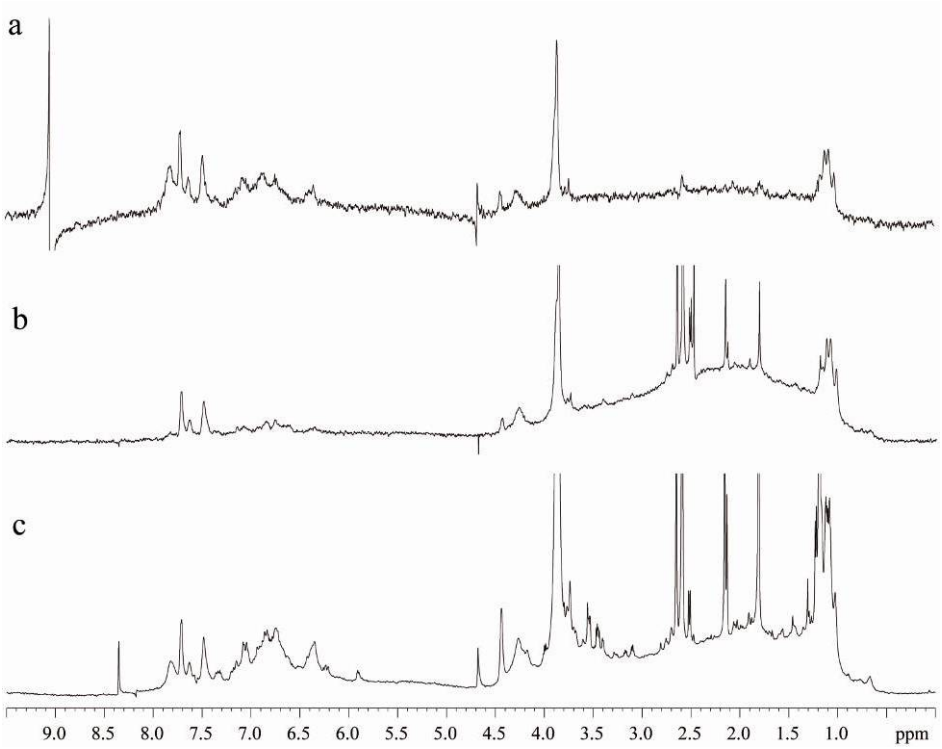


Figure 47S. DF-STD spectra of the **29** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (9.0 ppm) and deoxyribose/backbone (2.5 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

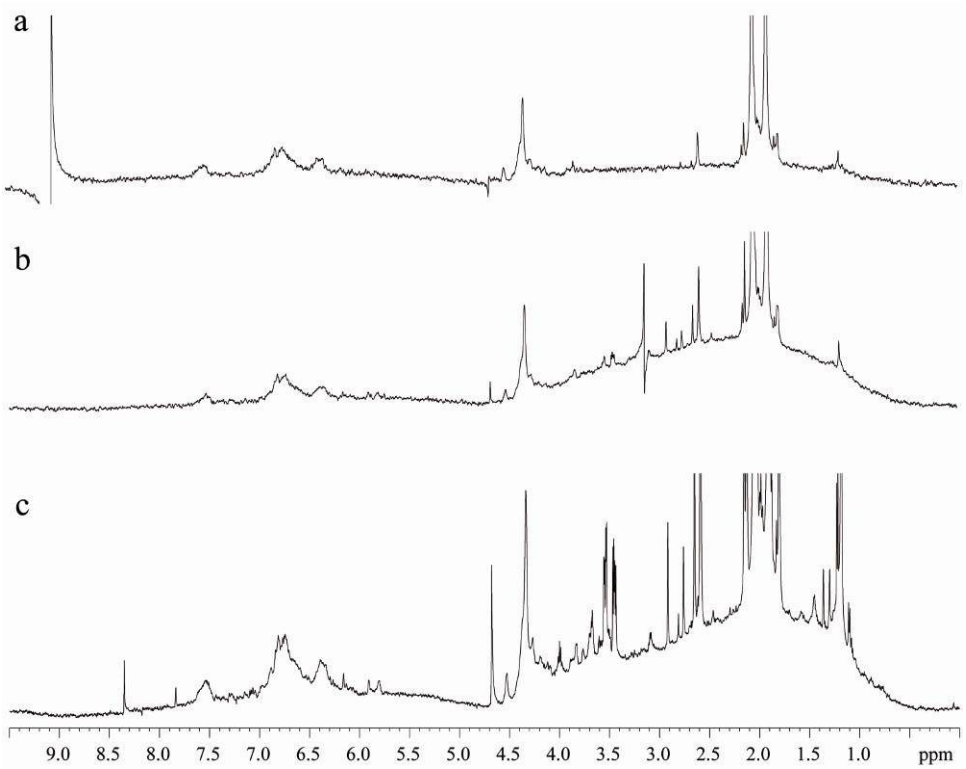


Figure 48S. DF-STD spectra of the **30** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (9.0 ppm) and deoxyribose/backbone (3.2 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

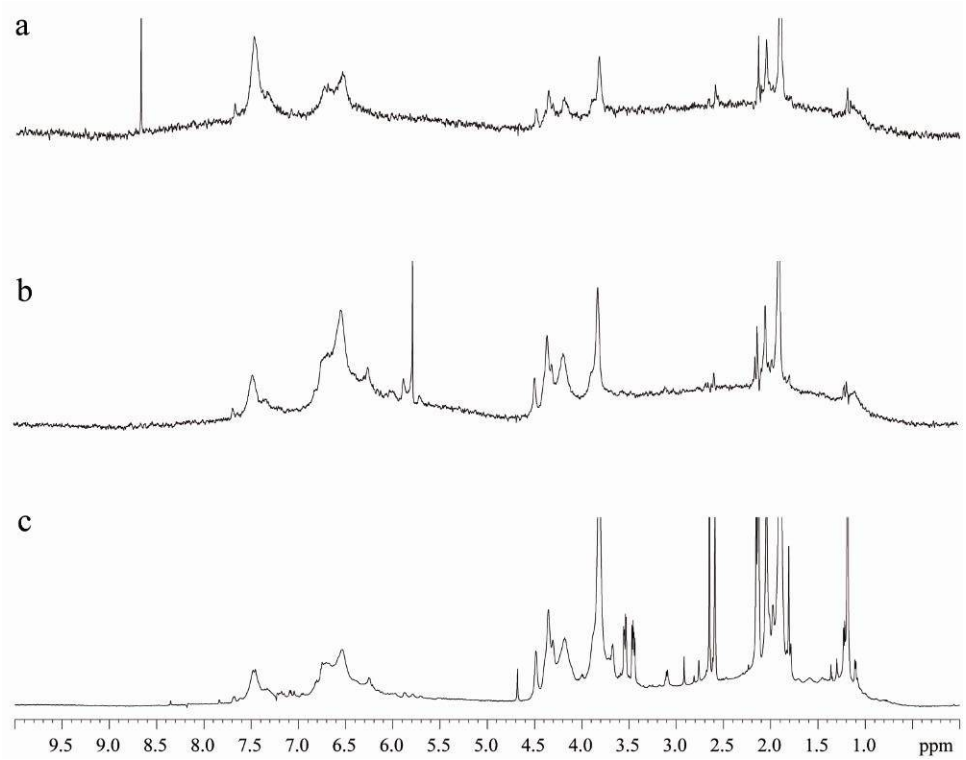


Figure 49S. DF-STD spectra of the **31** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (8.7 ppm) and deoxyribose/backbone (5.8 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

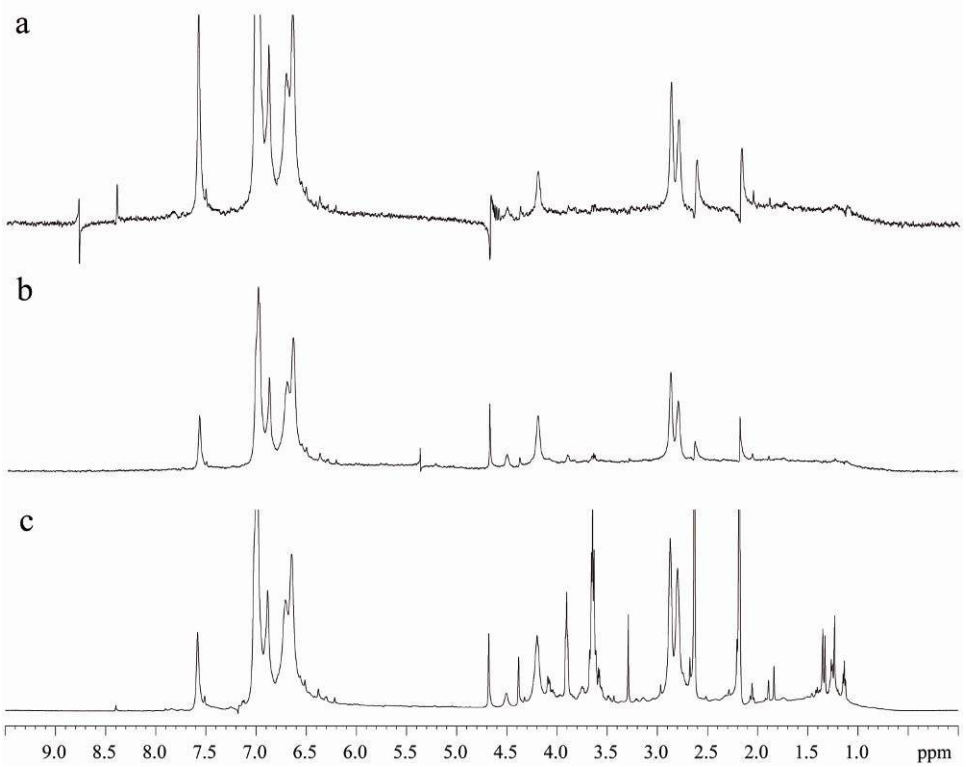


Figure 50S. DF-STD spectra of the **32** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (8.8 ppm) and deoxyribose/backbone (5.4 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

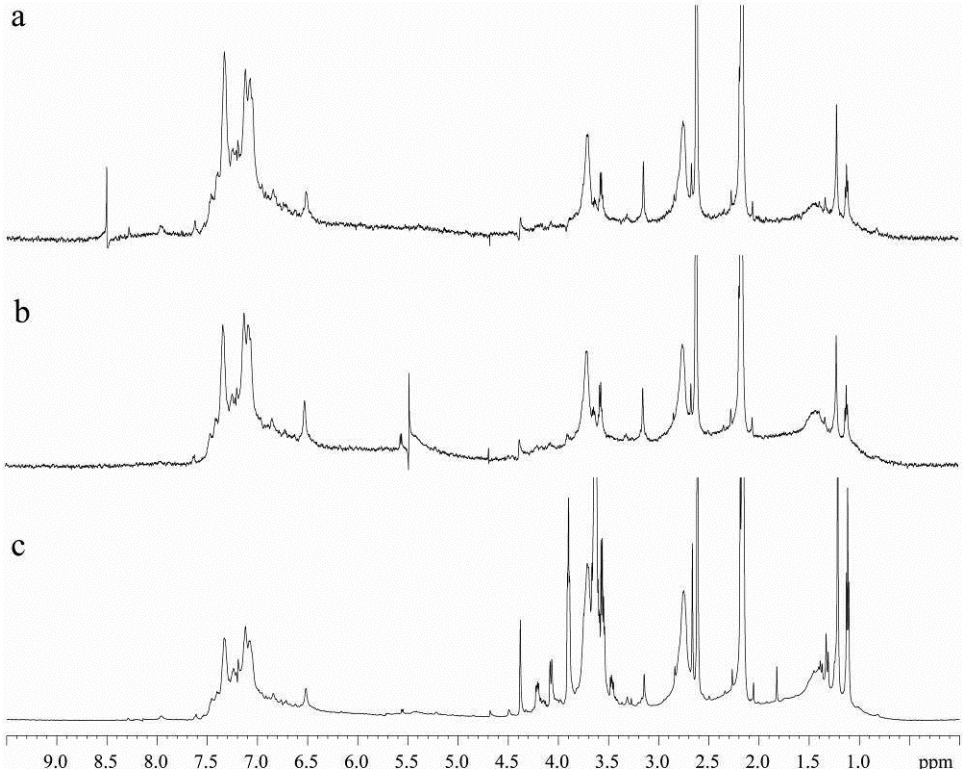


Figure 51S. DF-STD spectra of the **33** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (8.5 ppm) and deoxyribose/backbone (5.0 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

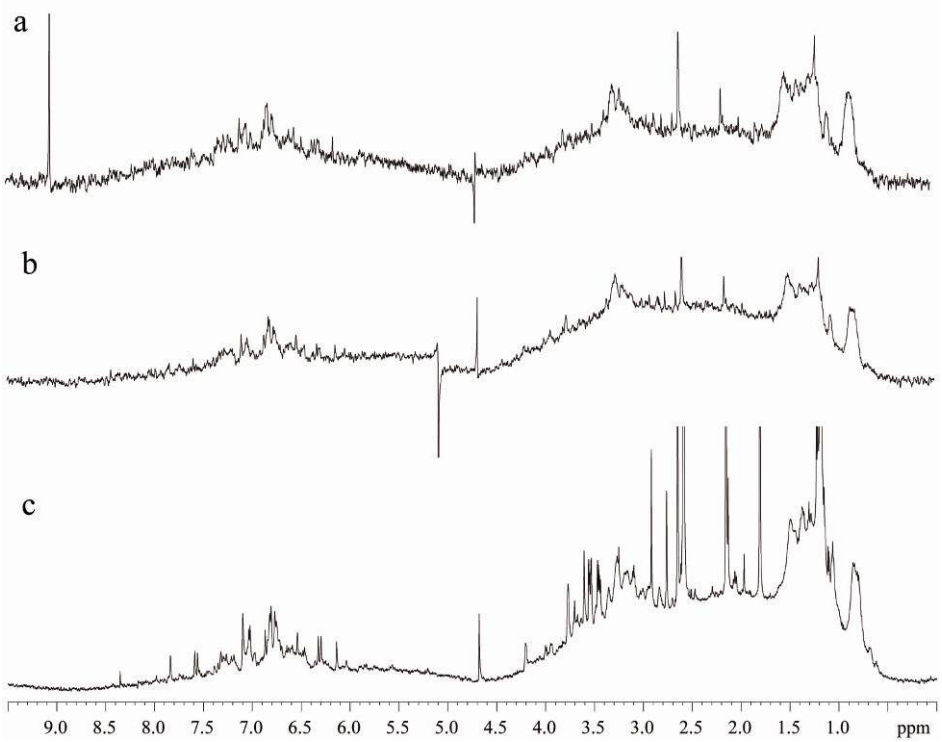


Figure 52S. DF-STD spectra of the **34** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (9.0 ppm) and deoxyribose/backbone (5.1 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

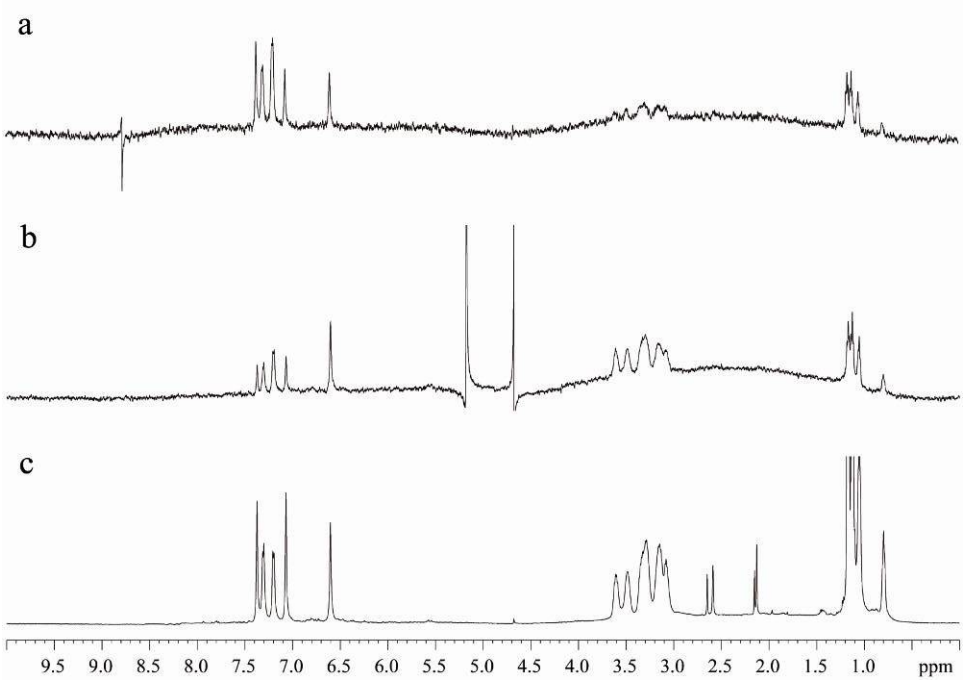


Figure 53S. DF-STD spectra of the **36** – DNA complex. a, b) STD spectra recorded upon saturation in the aromatic (8.8 ppm) and deoxyribose/backbone (5.4 ppm) spectral regions, respectively. c) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

Table S1: COSY and HMBC correlations of **30**

H	**δ_H**	**COSY**	**HMBC**
H-3	8.21		166.35, 124.01, 122.14, 121.17
H-4	7.53	7.35	142.74, 129.77, 124.01
H-5	7.35	7.53	137.45, 127.38
H-8	6.73		110.66, 147.62, 148.96, 142.44
H-11	7.25		125.06, 147.62, 148.96, 142.44
H-1"	4.54	4.43	166.35, 62.56
H-2"	4.43	4.54	170.78, 63.80
H-4"	1.98		170.78
H-1"'	4.64	4.43	170.45
H-2"'	4.43	4.64	170.78
H-4"'	2.07		170.78

Table S2: HMBC correlations of **31**

H	**δ_H**	**HMBC**
H-3	8.25	166.6, 124.0, 122.1, 121.3
H-4	7.52	142.7, 129.8, 124.0
H-5	7.34	137.5, 127.5
H-8	6.73	110.7, 147.63, 149.0, 142.5
H-11	7.25	125.0, 147.6, 149.0, 142.5
H-1''	4.39	166.6, 60.7
H-2''	3.90	
H-1'''	4.64	170.7
H-2'''	4.43	170.8, 60.7
H-4'''	1.98	170.8

Table S3: NMR data of **32**

H	**δ_H**	**HMBC**
H-3	7.94	166.3, 123.3, 120.9, 118.5
H-4	7.32	141.7, 128.6, 123.3,
H-5	7.21	136.9, 126.6
H-8	6.71	148.3, 147.0, 141.8, 109.6
H-11	7.10	148.3, 147.0, 141.7, 155.7, 155.5, 124.7, 124.5, 33.8, 33.3
H-1"	4.33	166.4, 129.6, 33.8
H-2"	2.97	129.6, 66.0
H-1"'	4.56	171.6, 129.7, 33.3
H-2"'	2.93	129.7, 66.8
H-2^{IV}-6^{IV}	7.10	148.3, 147.0, 141.8, 155.7, 155.5, 124.7, 124.5, 33.8, 33.3
H-3^{IV}-5^{IV}	6.69	
H-2^{V}-6^{V}	7.10	148.3, 147.0, 141.8, 155.7, 155.5, 124.7, 124.5, 33.8, 33.3
H-3^{V}-5^{V}	6.75	

Table S4: HMBC correlations of **33**

H	**δ_H**	**HMBC**
H-3	7.56	123.8, 121.3, 169.7,124.1, 138.1, 138.2, 136.3, 136.7, 122.0, 122.6,
H-4	7.13	141.7, 138.1, 138.2, 130.1, 130.2, 137.8
H-5	7.13	141.7, 138.1, 138.2,130.1, 130.2, 137.8
H-8	6.61	148.4, 149.4, 142.9, 111.6
H-11	7.30	142.9, 149.4,148.4
H-1"	3.74	136.7, 136.3
H-2"	2.79	136.7, 136.3, 130.1, 130.0
H-1"'	3.74	136.7, 136.3
H-2"'	2.79	136.7,136.3, 130.1, 130.0
$H\text{-}2^{IV}\text{-}6^{IV}$	7.13	141.7, 138.1, 138.2, 130.1, 130.2, 137.8, 128.2, 124.1
$H\text{-}3^{IV}\text{-}5^{IV}$	7.56	123.8, 121.3, 169.7, 124.1, 138.1, 138.2, 136.3, 136.7, 122.0, 122.6
$H\text{-}2^{V}\text{-}6^{V}$	7.13	141.7, 138.1, 138.2, 130.1, 130.2,137.8, 128.2, 124.1
$H\text{-}3^{V}\text{-}5^{V}$	7.56	123.8, 121.3, 169.7, 124.1, 138.1, 138.2, 136.3, 136.7, 122.0, 122.6

Table S5: HMBC correlations of **34**

H	**δ_H**	**HMBC**
H-3	7.61	124.7, 123.2, 120.7, 168.7
H-4	7.30	140.0, 123.2, 125.6
H-5	7.20	137.5, 127.0
H-8	6.62	148.5, 147.5, 142.3, 111.8
H-11	7.51	148.5, 147.5, 142.3, 124.1
H-1''	3.43	171.4, 20.9
H-2''	1.62	14.1
H-3''	1.46	40.5
H-4''	0.94	32.4
H-1'''	3.74	168.7, 20.7
H-2'''	1.62	14.1
H-3'''	1.46	40.1
H-4'''	0.94	31.5
NH-3'	7.38	
NH-3''	7.65	

Table S6: COSY correlations of **35**

H	**δ_H**	**COSY**
H-3	7.42	
H-4	7.26	7.19
H-5	7.19	7.26
H-8	6.69	
H-11	7.36	
H-1"	3.55	2.82
H-2"	2.82	3.55
H-1"'	3.55	2.82
H-2"'	2.82	3.55
$H\text{-}2^{IV}\text{-}6^{IV}$	7.08	6.70
$H\text{-}3^{IV}\text{-}5^{IV}$	6.70	7.08
$H\text{-}2^{V}\text{-}6^{V}$	7.13	6.75
$H\text{-}3^{V}\text{-}5^{V}$	6.75	7.13

Table S7: COSY and HMBC correlations of **36**

H	**δ_H**	**COSY**	**HMBC**
H-3	7.37		169.8, 120.3, 133.7, 122.2
H-4	7.34	7.24	122.2, 122.4, 142.3
H-5	7.24	7.34	127.9, 137.4, 140.6
H-8	6.67		148.4, 147.3, 142.3, 111.6
H-11	7.44		148.4, 147.3, 142.3, 123.1
H-1''	3.40	1.13	169.8, 13.9
H-2''	1.13	3.40	
H-3''	3.58	1.19	169.8, 12.8
H-4''	1.19	3.58	
H-1'''	3.74	1.23	170.2, 12.1
H-2'''	1.23	3.74	
H-3'''	3.19	0.92	170.2, 13.2
H-4'''	0.92	3.19	
-OH	8.41		
-OH	3.01		

Table S8: Binding energies calculated by the software Autodock 4.2, for **12**, **13** and **27 – 36**, interacting with two DNA models A and B.

	Binding Energy (kcal/mol)	
compound	**Model A**	**Model B**
12	-8.14[a]	-7.95[a]
13	-10.94[a]	-10.01[a]
27	-8.54	-8.30
28	-9.16	-9.05
29	-9.03	-8.46
30	-9.83	-8.48
31	-9.49	-8.06
32	-9.95	-8.43
33	-10.36	-10.38
34	-8.54	-8.43
35	-10.6	-10.34
36	-8.80	-8.13

[a]Binding energies values recalculated by Autodock 4.2, are slightly different with respect to our previous work[14] where they were calculated with Autodock 3.0.5.

Three dimensional coordinates of **Model A**, used in docking calculations.

Model A			
ATOM	**X**	**Y**	**Z**
O	-6.421	-6.784	-2.970
H	-6.364	-5.835	-3.102
P	-6.247	-7.119	-1.410
O	-6.332	-8.579	-1.181
O	-7.183	-6.289	-0.619
O	-4.746	-6.619	-1.169
C	-3.755	-6.874	-2.183
C	-2.383	-6.991	-1.549
O	-1.805	-5.659	-1.426
C	-2.354	-7.550	-0.126

O	-1.071	-8.082	0.190
C	-2.576	-6.304	0.731
C	-1.845	-5.233	-0.073
N	-2.504	-3.898	-0.029
C	-3.846	-3.589	0.016
N	-4.097	-2.303	0.046
C	-2.832	-1.717	0.020
C	-2.458	-0.349	0.035
O	-3.178	0.645	0.075
N	-1.065	-0.199	-0.003
C	-0.153	-1.235	-0.049
N	1.134	-0.882	-0.079
N	-0.505	-2.519	-0.062
C	-1.854	-2.682	-0.026
H	-0.719	0.719	0.005
H	1.385	0.077	-0.068
H	1.809	-1.550	-0.113
H	-3.992	-7.804	-2.698
H	-3.749	-6.053	-2.900
H	-1.730	-7.572	-2.200
H	-3.034	-8.398	-0.054
H	-3.645	-6.112	0.825
H	-2.147	-6.462	1.720
H	-0.831	-5.052	0.282
H	-4.581	-4.380	0.023
P	-0.659	-8.270	1.732
O	0.133	-9.512	1.880
O	-1.853	-8.163	2.599
O	0.284	-6.997	1.952
C	1.177	-6.598	0.894
C	2.397	-5.912	1.475
O	2.102	-4.497	1.655
C	2.830	-6.388	2.861
O	4.200	-6.082	3.105
C	1.978	-5.529	3.795
C	1.902	-4.211	3.031
N	0.595	-3.511	3.173
C	0.605	-2.119	3.208
O	1.689	-1.528	3.120
N	-0.576	-1.462	3.337
C	-1.727	-2.140	3.428
N	-2.853	-1.453	3.552
C	-1.759	-3.572	3.394
C	-0.568	-4.209	3.265
H	-2.829	-0.466	3.577

H	-3.700	-1.919	3.619
H	1.493	-7.478	0.334
H	0.662	-5.908	0.225
H	3.226	-5.985	0.770
H	2.774	-7.476	2.907
H	1.005	-5.999	3.934
H	2.477	-5.435	4.760
H	2.643	-3.484	3.363
H	-2.702	-4.093	3.469
H	-0.554	-5.288	3.236
P	4.729	-6.016	4.621
O	6.108	-6.550	4.690
O	3.744	-6.663	5.516
O	4.745	-4.438	4.886
C	5.178	-3.558	3.832
C	5.782	-2.299	4.422
O	4.714	-1.340	4.679
C	6.475	-2.465	5.774
O	7.407	-1.413	6.006
C	5.323	-2.306	6.767
C	4.448	-1.269	6.071
N	2.988	-1.485	6.274
C	2.288	-2.667	6.378
N	0.999	-2.510	6.554
C	0.832	-1.127	6.568
C	-0.345	-0.350	6.725
O	-1.501	-0.729	6.888
N	-0.062	1.023	6.677
C	1.193	1.572	6.500
N	1.251	2.905	6.484
N	2.296	0.842	6.353
C	2.039	-0.492	6.398
H	-0.822	1.634	6.778
H	0.424	3.439	6.595
H	2.086	3.343	6.365
H	5.928	-4.062	3.222
H	4.326	-3.288	3.209
H	6.460	-1.846	3.699
H	7.075	-3.375	5.766
H	4.824	-3.265	6.901
H	5.714	-1.962	7.725
H	4.628	-0.253	6.424
H	2.810	-3.610	6.313
P	7.882	-1.103	7.510
O	9.315	-0.734	7.505

O	7.509	-2.220	8.406
O	6.993	0.183	7.849
C	6.774	1.171	6.824
C	6.565	2.534	7.453
O	5.156	2.686	7.792
C	7.301	2.778	8.771
O	7.460	4.172	9.019
C	6.330	2.218	9.809
C	4.977	2.563	9.195
N	3.929	1.533	9.439
C	2.620	1.970	9.626
O	2.384	3.184	9.582
N	1.650	1.047	9.848
C	1.946	-0.258	9.887
N	0.964	-1.119	10.108
C	3.286	-0.729	9.697
C	4.240	0.210	9.476
H	0.042	-0.793	10.240
H	1.151	-2.070	10.139
H	7.641	1.210	6.165
H	5.890	0.904	6.245
H	6.812	3.311	6.729
H	8.317	2.389	8.698
H	6.489	1.145	9.915
H	6.501	2.706	10.768
H	4.554	3.487	9.590
H	3.496	-1.788	9.733
H	5.262	-0.109	9.329
P	7.727	4.672	10.523
O	8.663	5.818	10.507
O	8.134	3.521	11.361
O	6.270	5.168	10.959
C	5.455	5.868	10.000
C	4.516	6.821	10.713
O	3.310	6.096	11.093
C	5.035	7.408	12.025
O	4.353	8.615	12.352
C	4.640	6.346	13.051
C	3.313	5.843	12.490
N	3.091	4.385	12.696
C	4.005	3.354	12.683
N	3.479	2.173	12.900
C	2.121	2.439	13.069
C	1.042	1.557	13.333
O	1.063	0.337	13.476

N	-0.173	2.249	13.430
C	-0.325	3.615	13.290
N	-1.569	4.081	13.419
N	0.688	4.442	13.043
C	1.875	3.786	12.946
H	-0.973	1.713	13.612
H	-2.316	3.456	13.604
H	-1.739	5.012	13.332
H	6.095	6.436	9.324
H	4.869	5.150	9.427
H	4.217	7.616	10.030
H	6.079	7.699	11.906
H	5.408	5.574	13.089
H	4.540	6.808	14.033
H	2.448	6.322	12.949
H	5.049	3.561	12.505
P	4.372	9.139	13.871
O	4.464	10.616	13.879
O	5.411	8.426	14.647
O	2.920	8.684	14.367
C	1.807	8.796	13.461
C	0.523	9.007	14.239
O	-0.016	7.708	14.620
C	0.664	9.762	15.561
O	-0.577	10.338	15.958
C	1.009	8.649	16.550
C	0.199	7.478	16.004
N	0.877	6.160	16.153
C	0.082	5.047	16.412
O	-1.143	5.197	16.507
N	0.680	3.836	16.551
C	2.009	3.716	16.441
N	2.545	2.513	16.585
C	2.846	4.848	16.174
C	2.227	6.048	16.040
H	1.968	1.734	16.770
H	3.505	2.398	16.508
H	1.964	9.643	12.793
H	1.722	7.881	12.873
H	-0.215	9.492	13.600
H	1.336	10.609	15.426
H	2.084	8.469	16.535
H	0.705	8.948	17.554
H	-0.761	7.354	16.506
H	3.915	4.722	16.090

H	2.826	6.924	15.839
P	-0.890	11.121	17.343
O	-1.808	12.323	16.994
O	0.449	11.389	18.079
O	-1.754	10.083	18.242
C	-3.200	10.066	18.199
C	-3.864	8.886	18.951
O	-3.139	7.710	18.633
C	-3.963	8.991	20.494
O	-5.273	8.602	20.979
C	-2.930	7.968	20.945
C	-2.977	6.945	19.809
N	-1.704	6.201	19.731
C	-0.455	6.737	19.571
N	0.517	5.870	19.669
C	-0.142	4.664	19.894
C	0.391	3.359	20.076
O	1.571	3.013	20.090
N	-0.618	2.433	20.284
C	-1.973	2.693	20.276
N	-2.768	1.653	20.507
N	-2.463	3.926	20.127
C	-1.503	4.853	19.918
H	-0.343	1.476	20.413
H	-2.403	0.731	20.622
H	-3.759	1.780	20.508
H	-3.595	11.005	18.591
H	-3.495	9.984	17.152
H	-4.880	8.786	18.563
H	-3.703	10.000	20.817
H	-1.961	8.465	20.994
H	-3.163	7.518	21.910
H	-3.833	6.281	19.937
H	-0.355	7.801	19.401
P	-5.852	9.033	22.430
O	-7.348	9.398	22.229
O	-4.902	10.102	23.032
O	-5.793	7.756	23.414
C	-6.835	6.757	23.452
C	-6.571	5.656	24.504
O	-5.170	5.407	24.540
C	-7.017	5.952	25.964
O	-7.923	4.974	26.504
C	-5.692	5.888	26.709
C	-4.876	4.947	25.838

N	-3.458	5.064	26.195
C	-2.652	3.949	26.385
O	-3.132	2.824	26.516
N	-1.302	4.133	26.378
C	-0.789	5.363	26.233
N	0.536	5.493	26.228
C	-1.611	6.518	26.075
C	-2.937	6.311	26.090
H	1.129	4.699	26.343
H	0.937	6.407	26.121
H	-7.803	7.216	23.657
H	-6.877	6.286	22.469
H	-7.083	4.748	24.181
H	-7.457	6.947	26.056
H	-5.380	6.926	26.750
H	-5.654	5.519	27.726
H	-5.209	3.925	25.875
H	-1.182	7.501	25.954
H	-3.595	7.154	25.948
P	-8.149	4.809	28.089
O	-9.613	4.446	28.350
O	-7.696	6.101	28.794
O	-7.175	3.615	28.485
C	-7.092	2.489	27.613
C	-6.736	1.227	28.388
O	-5.324	1.160	28.550
C	-7.300	1.182	29.807
O	-7.388	-0.160	30.264
C	-6.216	1.888	30.613
C	-4.941	1.470	29.883
N	-3.908	2.531	29.811
C	-4.052	3.894	29.744
N	-2.928	4.557	29.677
C	-1.960	3.563	29.803
C	-0.544	3.663	29.871
O	0.159	4.669	29.768
N	0.050	2.409	29.917
C	-0.624	1.208	30.058
N	0.151	0.121	30.084
N	-1.952	1.114	29.956
C	-2.548	2.327	29.906
H	1.048	2.378	29.998
H	1.141	0.190	30.165
H	-0.284	-0.771	30.195
H	-8.031	2.351	27.079

H	-6.304	2.659	26.888
H	-7.075	0.362	27.817
H	-8.328	1.543	29.822
H	-6.387	2.964	30.595
H	-6.240	1.541	31.649
H	-4.449	0.614	30.341
H	-5.042	4.324	29.669
P	-7.438	-0.465	31.844
O	-8.408	-1.627	32.115
O	-7.789	0.845	32.586
O	-5.938	-0.890	32.140
C	-5.260	-1.711	31.192
C	-4.205	-2.561	31.894
O	-3.002	-1.813	32.012
C	-4.558	-2.978	33.320
O	-3.823	-4.138	33.695
C	-4.045	-1.799	34.142
C	-2.812	-1.369	33.350
N	-2.580	0.091	33.342
C	-1.272	0.546	33.380
O	-0.349	-0.279	33.362
N	-1.037	1.884	33.345
C	-2.063	2.742	33.342
N	-1.779	4.047	33.284
C	-3.427	2.307	33.295
C	-3.623	0.971	33.328
H	-0.830	4.352	33.336
H	-2.526	4.706	33.307
H	-5.975	-2.358	30.682
H	-4.765	-1.073	30.460
H	-4.005	-3.442	31.281
H	-5.604	-3.281	33.378
H	-4.812	-1.026	34.184
H	-3.813	-2.131	35.154
H	-1.890	-1.793	33.751
H	-4.223	3.031	33.293
H	-4.636	0.596	33.313
P	-3.588	-4.425	35.250
O	-3.667	-5.946	35.484
O	-4.573	-3.613	36.113
O	-2.097	-3.913	35.502
H	-1.863	-4.048	36.422
P	6.296	4.986	-1.901
O	7.756	5.022	-2.141
O	5.493	5.958	-2.676

O	5.741	3.507	-2.150
H	4.794	3.489	-1.993
P	2.360	8.887	1.487
O	3.515	9.777	1.229
O	1.118	9.218	0.754
O	2.771	7.369	1.196
C	3.576	6.666	2.161
C	4.411	5.607	1.469
O	3.623	4.387	1.352
C	4.832	5.926	0.034
O	5.974	5.165	-0.347
C	3.639	5.434	-0.785
C	3.191	4.213	0.011
N	1.714	4.015	0.024
C	1.234	2.708	0.018
O	2.046	1.774	0.003
N	-0.108	2.506	0.030
C	-0.953	3.544	0.047
N	-2.254	3.295	0.058
C	-0.481	4.897	0.054
C	0.865	5.076	0.041
H	-2.579	2.363	0.052
H	-2.888	4.029	0.072
H	4.237	7.370	2.666
H	2.928	6.187	2.895
H	5.284	5.375	2.079
H	5.154	6.965	-0.028
H	2.881	6.216	-0.830
H	3.967	5.188	-1.795
H	3.591	3.278	-0.382
H	-1.185	5.715	0.068
H	1.257	6.082	0.045
P	-2.919	9.674	5.216
O	-2.514	11.075	4.964
O	-4.164	9.235	4.547
O	-1.721	8.686	4.830
C	-0.602	8.563	5.728
C	0.650	8.205	4.951
O	0.711	6.757	4.798
C	0.720	8.740	3.521
O	2.066	8.796	3.059
C	-0.012	7.663	2.720
C	0.381	6.392	3.467
N	-0.702	5.371	3.522
C	-2.064	5.551	3.626

N	-2.750	4.434	3.651
C	-1.773	3.444	3.557
C	-1.903	2.031	3.534
O	-2.924	1.351	3.592
N	-0.654	1.404	3.429
C	0.562	2.056	3.355
N	1.640	1.276	3.258
N	0.682	3.382	3.377
C	-0.521	4.006	3.478
H	-0.652	0.424	3.406
H	1.539	0.290	3.242
H	2.505	1.666	3.205
H	-0.444	9.510	6.244
H	-0.806	7.780	6.458
H	1.529	8.511	5.517
H	0.374	9.773	3.501
H	-1.084	7.858	2.744
H	0.337	7.677	1.688
H	1.225	5.875	3.011
H	-2.475	6.549	3.678
P	-7.432	7.055	9.087
O	-7.946	8.431	8.906
O	-8.208	5.986	8.419
O	-5.903	6.983	8.623
C	-4.884	7.517	9.490
C	-3.703	7.997	8.669
O	-2.805	6.873	8.435
C	-4.033	8.517	7.271
O	-3.004	9.375	6.787
C	-4.025	7.243	6.426
C	-2.921	6.429	7.092
N	-3.187	4.963	7.112
C	-2.100	4.104	6.972
O	-0.969	4.589	6.839
N	-2.321	2.765	6.987
C	-3.560	2.280	7.134
N	-3.724	0.966	7.143
C	-4.693	3.146	7.280
C	-4.449	4.481	7.261
H	-2.943	0.370	7.041
H	-4.611	0.588	7.250
H	-5.291	8.355	10.056
H	-4.550	6.742	10.180
H	-3.148	8.745	9.234
H	-4.923	9.144	7.316

H	-5.002	6.764	6.481
H	-3.803	7.496	5.389
H	-1.958	6.528	6.592
H	-5.681	2.727	7.397
H	-5.279	5.164	7.368
P	-9.389	2.217	12.980
O	-10.617	3.038	12.875
O	-9.431	0.908	12.291
O	-8.130	3.058	12.466
C	-7.570	4.072	13.323
C	-6.932	5.164	12.487
O	-5.561	4.779	12.176
C	-7.573	5.418	11.123
O	-7.263	6.723	10.645
C	-6.869	4.402	10.224
C	-5.465	4.373	10.819
N	-4.827	3.027	10.783
C	-5.405	1.785	10.932
N	-4.557	0.789	10.848
C	-3.331	1.415	10.627
C	-2.038	0.857	10.453
O	-1.703	-0.325	10.455
N	-1.073	1.854	10.255
C	-1.324	3.212	10.230
N	-0.265	4.000	10.027
N	-2.537	3.735	10.394
C	-3.485	2.780	10.586
H	-0.148	1.554	10.125
H	0.634	3.600	9.906
H	-0.373	4.943	10.001
H	-8.359	4.505	13.937
H	-6.812	3.625	13.967
H	-6.888	6.086	13.066
H	-8.659	5.407	11.224
H	-7.380	3.442	10.289
H	-6.888	4.754	9.193
H	-4.766	5.024	10.293
H	-6.468	1.701	11.101
P	-7.876	-2.942	16.627
O	-9.354	-3.005	16.608
O	-7.178	-3.999	15.862
O	-7.388	-1.502	16.129
C	-7.484	-0.382	17.030
C	-7.665	0.902	16.244
O	-6.352	1.413	15.871

C	-8.412	0.770	14.917
O	-8.960	2.020	14.510
C	-7.299	0.398	13.938
C	-6.116	1.187	14.489
N	-4.810	0.483	14.354
C	-3.679	1.254	14.100
O	-3.805	2.482	13.999
N	-2.480	0.632	13.973
C	-2.387	-0.699	14.090
N	-1.194	-1.259	13.958
C	-3.538	-1.512	14.351
C	-4.727	-0.869	14.474
H	-0.402	-0.698	13.776
H	-1.098	-2.221	14.039
H	-8.340	-0.520	17.691
H	-6.573	-0.314	17.624
H	-8.139	1.652	16.877
H	-9.273	0.115	15.048
H	-7.140	-0.680	13.959
H	-7.583	0.703	12.931
H	-5.968	2.142	13.984
H	-3.433	-2.583	14.441
H	-5.616	-1.450	14.671
P	-3.477	-6.354	20.005
O	-4.642	-7.267	20.014
O	-2.328	-6.786	19.177
O	-3.941	-4.888	19.561
C	-4.632	-4.057	20.513
C	-5.560	-3.101	19.790
O	-4.809	-1.911	19.412
C	-6.148	-3.612	18.475
O	-7.338	-2.908	18.136
C	-5.070	-3.241	17.456
C	-4.545	-1.923	18.017
N	-3.081	-1.730	17.822
C	-2.069	-2.664	17.845
N	-0.876	-2.163	17.636
C	-1.114	-0.801	17.462
C	-0.208	0.260	17.202
O	1.012	0.215	17.069
N	-0.875	1.488	17.096
C	-2.239	1.668	17.225
N	-2.680	2.921	17.089
N	-3.088	0.672	17.469
C	-2.457	-0.527	17.574

H	-0.322	2.277	16.916
H	-2.039	3.655	16.907
H	-3.608	3.109	17.168
H	-5.217	-4.684	21.186
H	-3.907	-3.484	21.090
H	-6.355	-2.784	20.466
H	-6.460	-4.649	18.594
H	-4.313	-4.024	17.426
H	-5.523	-3.135	16.470
H	-5.003	-1.050	17.553
H	-2.298	-3.704	18.025
P	2.208	-6.377	24.881
O	1.719	-7.779	25.335
O	3.499	-6.282	24.025
O	1.029	-5.709	24.004
C	-0.365	-6.050	24.178
C	-1.295	-5.277	23.212
O	-0.704	-4.002	22.984
C	-1.567	-5.911	21.818
O	-2.959	-6.131	21.517
C	-1.006	-4.849	20.882
C	-1.120	-3.578	21.708
N	-0.250	-2.550	21.125
C	-0.693	-1.253	20.903
O	-1.889	-0.968	20.939
N	0.247	-0.290	20.687
C	1.547	-0.613	20.650
N	2.428	0.362	20.441
C	2.007	-1.949	20.841
C	1.063	-2.880	21.049
H	2.129	1.303	20.299
H	3.406	0.141	20.410
H	-0.521	-7.121	24.043
H	-0.643	-5.787	25.200
H	-2.261	-5.138	23.703
H	-1.018	-6.847	21.694
H	-0.007	-5.207	20.658
H	-1.479	-4.666	19.927
H	-2.124	-3.218	21.835
H	3.058	-2.191	20.815
H	1.366	-3.901	21.223
P	7.619	-3.327	28.929
O	8.087	-4.752	29.327
O	8.494	-2.496	27.953
O	6.139	-3.455	28.280

C	5.290	-4.596	28.550
C	3.845	-4.475	28.005
O	3.394	-3.162	28.295
C	3.638	-4.736	26.492
O	2.430	-5.495	26.225
C	3.471	-3.318	25.963
C	2.774	-2.636	27.141
N	2.964	-1.172	27.089
C	4.150	-0.491	27.009
N	4.017	0.797	26.834
C	2.637	0.985	26.811
C	1.883	2.180	26.655
O	2.301	3.324	26.490
N	0.524	1.919	26.684
C	-0.064	0.686	26.881
N	-1.392	0.663	26.861
N	0.653	-0.433	27.003
C	1.985	-0.212	26.983
H	-0.095	2.705	26.592
H	-1.929	1.500	26.768
H	-1.872	-0.202	27.004
H	5.746	-5.502	28.151
H	5.217	-4.700	29.634
H	3.231	-5.192	28.552
H	4.517	-5.227	26.073
H	4.461	-2.899	25.788
H	2.878	-3.269	25.049
H	1.716	-2.905	27.147
H	5.082	-1.037	27.074
P	9.708	2.317	31.695
O	10.997	1.507	31.495
O	9.653	3.542	30.784
O	8.430	1.415	31.430
C	8.024	0.545	32.489
C	7.303	-0.666	31.898
O	5.932	-0.336	31.717
C	7.782	-1.111	30.507
O	7.431	-2.485	30.300
C	6.937	-0.228	29.595
C	5.616	-0.130	30.356
N	4.950	1.183	30.204
C	3.559	1.204	30.196
O	2.965	0.133	30.244
N	2.943	2.397	30.019
C	3.636	3.534	29.967

N	2.965	4.671	29.807
C	5.068	3.538	29.983
C	5.671	2.338	30.118
H	1.960	4.674	29.810
H	3.461	5.536	29.757
H	8.896	0.211	33.053
H	7.345	1.074	33.159
H	7.370	-1.488	32.615
H	8.871	-1.070	30.480
H	7.433	0.729	29.448
H	6.833	-0.717	28.625
H	4.882	-0.860	30.021
H	5.602	4.475	29.912
H	6.751	2.302	30.145
P	8.667	7.919	34.813
O	10.177	8.016	34.536
O	7.853	8.910	33.982
O	8.127	6.447	34.535
C	8.368	5.475	35.551
C	8.442	4.089	34.919
O	7.130	3.554	34.795
C	9.012	4.058	33.502
O	9.519	2.763	33.197
C	7.772	4.300	32.645
C	6.683	3.597	33.453
N	5.368	4.278	33.403
C	5.084	5.622	33.356
N	3.808	5.900	33.325
C	3.196	4.650	33.352
C	1.819	4.306	33.340
O	0.838	5.045	33.297
N	1.644	2.929	33.379
C	2.650	1.994	33.456
N	2.281	0.716	33.430
N	3.960	2.311	33.416
C	4.140	3.655	33.400
H	0.701	2.584	33.373
H	1.299	0.476	33.461
H	2.940	-0.019	33.512
H	9.303	5.692	36.068
H	7.548	5.485	36.270
H	9.023	3.436	35.573
H	9.876	4.718	33.425
H	7.604	5.372	32.546
H	7.920	3.869	31.654

H	6.487	2.584	33.096
H	5.888	6.345	33.346
O	8.313	8.103	36.355
H	7.360	8.061	36.457

Three dimensional coordinates of **Model B**, used in docking calculations.

Model B			
ATOM	**X**	**Y**	**Z**
P	-6.247	-7.119	-1.410
O	-6.332	-8.579	-1.181
O	-7.183	-6.289	-0.619
O	-4.746	-6.619	-1.169
C	-3.755	-6.874	-2.183
C	-2.383	-6.991	-1.549
O	-1.805	-5.659	-1.426
C	-2.354	-7.550	-0.126
O	-1.071	-8.082	0.190
C	-2.576	-6.304	0.731
C	-1.845	-5.233	-0.073
N	-2.504	-3.898	-0.029
C	-3.846	-3.589	0.016
N	-4.097	-2.303	0.046
C	-2.832	-1.717	0.020
C	-2.458	-0.349	0.035
O	-3.178	0.645	0.075
N	-1.065	-0.199	-0.003
C	-0.153	-1.235	-0.049
N	1.134	-0.882	-0.079
N	-0.505	-2.519	-0.062
C	-1.854	-2.682	-0.026
H	-0.719	0.719	0.005
H	1.385	0.077	-0.068
H	1.809	-1.550	-0.113
H	-3.992	-7.804	-2.698
H	-3.749	-6.053	-2.900
H	-1.730	-7.572	-2.200
H	-3.034	-8.398	-0.054
H	-3.645	-6.112	0.825
H	-2.147	-6.462	1.720
H	-0.831	-5.052	0.282
H	-4.581	-4.380	0.023

P	-0.659	-8.270	1.732
O	0.133	-9.512	1.880
O	-1.853	-8.163	2.599
O	0.284	-6.997	1.952
C	1.177	-6.598	0.894
C	2.397	-5.912	1.475
O	2.102	-4.497	1.655
C	2.830	-6.388	2.861
O	4.200	-6.082	3.105
C	1.978	-5.529	3.795
C	1.902	-4.211	3.031
N	0.595	-3.511	3.173
C	0.605	-2.119	3.208
O	1.689	-1.528	3.120
N	-0.576	-1.462	3.337
C	-1.727	-2.140	3.428
N	-2.853	-1.453	3.552
C	-1.759	-3.572	3.394
C	-0.568	-4.209	3.265
H	-2.829	-0.466	3.577
H	-3.700	-1.919	3.619
H	1.493	-7.478	0.334
H	0.662	-5.908	0.225
H	3.226	-5.985	0.770
H	2.774	-7.476	2.907
H	1.005	-5.999	3.934
H	2.477	-5.435	4.760
H	2.643	-3.484	3.363
H	-2.702	-4.093	3.469
H	-0.554	-5.288	3.236
P	4.729	-6.016	4.621
O	6.108	-6.550	4.690
O	3.744	-6.663	5.516
O	4.745	-4.438	4.886
C	5.178	-3.558	3.832
C	5.782	-2.299	4.422
O	4.714	-1.340	4.679
C	6.475	-2.465	5.774
O	7.407	-1.413	6.006
C	5.323	-2.306	6.767
C	4.448	-1.269	6.071
N	2.988	-1.485	6.274
C	2.288	-2.667	6.378
N	0.999	-2.510	6.554
C	0.832	-1.127	6.568

C	-0.345	-0.350	6.725
O	-1.501	-0.729	6.888
N	-0.062	1.023	6.677
C	1.193	1.572	6.500
N	1.251	2.905	6.484
N	2.296	0.842	6.353
C	2.039	-0.492	6.398
H	-0.822	1.634	6.778
H	0.424	3.439	6.595
H	2.086	3.343	6.365
H	5.928	-4.062	3.222
H	4.326	-3.288	3.209
H	6.460	-1.846	3.699
H	7.075	-3.375	5.766
H	4.824	-3.265	6.901
H	5.714	-1.962	7.725
H	4.628	-0.253	6.424
H	2.810	-3.610	6.313
P	7.882	-1.103	7.510
O	9.315	-0.734	7.505
O	7.509	-2.220	8.406
O	6.993	0.183	7.849
C	6.774	1.171	6.824
C	6.565	2.534	7.453
O	5.156	2.686	7.792
C	7.301	2.778	8.771
O	7.460	4.172	9.019
C	6.330	2.218	9.809
C	4.977	2.563	9.195
N	3.929	1.533	9.439
C	2.620	1.970	9.626
O	2.384	3.184	9.582
N	1.650	1.047	9.848
C	1.946	-0.258	9.887
N	0.964	-1.119	10.108
C	3.286	-0.729	9.697
C	4.240	0.210	9.476
H	0.042	-0.793	10.240
H	1.151	-2.070	10.139
H	7.641	1.210	6.165
H	5.890	0.904	6.245
H	6.812	3.311	6.729
H	8.317	2.389	8.698
H	6.489	1.145	9.915
H	6.501	2.706	10.768

H	4.554	3.487	9.590
H	3.496	-1.788	9.733
H	5.262	-0.109	9.329
P	7.727	4.672	10.523
O	8.663	5.818	10.507
O	8.134	3.521	11.361
O	6.270	5.168	10.959
C	5.455	5.868	10.000
C	4.516	6.821	10.713
O	3.310	6.096	11.093
C	5.035	7.408	12.025
O	4.353	8.615	12.352
C	4.640	6.346	13.051
C	3.313	5.843	12.490
N	3.091	4.385	12.696
C	4.005	3.354	12.683
N	3.479	2.173	12.900
C	2.121	2.439	13.069
C	1.042	1.557	13.333
O	1.063	0.337	13.476
N	-0.173	2.249	13.430
C	-0.325	3.615	13.290
N	-1.569	4.081	13.419
N	0.688	4.442	13.043
C	1.875	3.786	12.946
H	-0.973	1.713	13.612
H	-2.316	3.456	13.604
H	-1.739	5.012	13.332
H	6.095	6.436	9.324
H	4.869	5.150	9.427
H	4.217	7.616	10.030
H	6.079	7.699	11.906
H	5.408	5.574	13.089
H	4.540	6.808	14.033
H	2.448	6.322	12.949
H	5.049	3.561	12.505
P	4.525	9.501	13.703
O	4.502	10.993	13.277
O	5.751	8.968	14.492
O	3.201	9.223	14.600
C	2.064	10.123	14.588
C	0.796	9.599	15.311
O	0.681	8.216	15.021
C	0.706	9.778	16.849
O	-0.591	10.272	17.270

C	0.878	8.350	17.350
C	0.294	7.531	16.194
N	0.882	6.168	16.167
C	0.081	5.062	16.403
O	-1.138	5.179	16.517
N	0.674	3.843	16.552
C	2.004	3.726	16.441
N	2.535	2.513	16.581
C	2.848	4.846	16.169
C	2.233	6.038	16.032
H	1.962	1.719	16.774
H	3.529	2.399	16.510
H	2.347	11.087	15.011
H	1.789	10.279	13.543
H	-0.060	10.118	14.875
H	1.508	10.429	17.198
H	1.944	8.176	17.494
H	0.352	8.159	18.286
H	-0.794	7.544	16.260
H	3.918	4.723	16.091
H	2.832	6.918	15.839
P	-0.863	10.952	18.717
O	-1.843	12.133	18.481
O	0.512	11.252	19.372
O	-1.608	9.887	19.676
C	-3.041	9.703	19.664
C	-3.541	8.724	20.752
O	-2.614	7.647	20.855
C	-3.740	9.305	22.179
O	-5.061	9.045	22.702
C	-2.676	8.540	22.955
C	-2.619	7.224	22.202
N	-1.411	6.497	22.588
C	-0.163	7.035	22.500
N	0.792	6.153	22.589
C	0.123	4.956	22.813
C	0.666	3.657	22.995
O	1.840	3.299	23.006
N	-0.346	2.726	23.189
C	-1.697	2.992	23.201
N	-2.497	1.950	23.411
N	-2.198	4.217	23.032
C	-1.237	5.153	22.840
H	-0.066	1.772	23.329
H	-2.130	1.028	23.539

H	-3.487	2.073	23.424
H	-3.552	10.657	19.797
H	-3.313	9.300	18.687
H	-4.503	8.325	20.422
H	-3.538	10.377	22.214
H	-1.771	9.133	22.852
H	-2.838	8.355	24.012
H	-3.476	6.596	22.347
H	-0.069	8.092	22.306
P	-5.415	9.128	24.274
O	-6.823	9.705	24.463
O	-4.319	9.930	24.993
O	-5.362	7.608	24.758
C	-5.936	6.615	23.910
C	-6.424	5.425	24.727
O	-5.337	4.538	24.974
C	-6.955	5.793	26.111
O	-7.822	4.777	26.594
C	-5.692	5.757	26.969
C	-4.892	4.636	26.312
N	-3.429	4.864	26.300
C	-2.592	3.772	26.464
O	-3.096	2.657	26.588
N	-1.249	3.961	26.443
C	-0.746	5.196	26.311
N	0.578	5.318	26.292
C	-1.585	6.341	26.137
C	-2.917	6.124	26.160
H	1.179	4.530	26.419
H	0.988	6.231	26.199
H	-6.755	7.031	23.325
H	-5.178	6.247	23.228
H	-7.191	4.900	24.154
H	-7.570	6.691	26.062
H	-5.194	6.726	26.916
H	-5.957	5.547	28.005
H	-5.017	3.678	26.818
H	-1.135	7.320	26.030
H	-3.580	6.968	26.041
P	-8.110	4.636	28.167
O	-9.575	4.267	28.432
O	-7.610	5.928	28.853
O	-7.117	3.439	28.562
C	-7.039	2.321	27.678
C	-6.690	1.056	28.460

O	-5.275	0.984	28.618
C	-7.253	1.007	29.880
O	-7.341	-0.341	30.333
C	-6.168	1.714	30.688
C	-4.898	1.300	29.946
N	-3.861	2.357	29.903
C	-4.010	3.721	29.808
N	-2.882	4.377	29.763
C	-1.909	3.388	29.878
C	-0.494	3.489	29.930
O	0.203	4.498	29.848
N	0.095	2.235	30.023
C	-0.576	1.033	30.115
N	0.195	-0.053	30.171
N	-1.907	0.941	30.044
C	-2.501	2.154	29.956
H	1.099	2.209	30.053
H	1.189	0.019	30.231
H	-0.236	-0.949	30.261
H	-7.983	2.179	27.153
H	-6.247	2.506	26.951
H	-7.030	0.189	27.891
H	-8.281	1.370	29.894
H	-6.342	2.790	30.664
H	-6.197	1.367	31.721
H	-4.405	0.444	30.411
H	-4.998	4.153	29.739
P	-7.391	-0.626	31.905
O	-8.356	-1.794	32.186
O	-7.734	0.663	32.678
O	-5.891	-1.071	32.225
C	-5.216	-1.883	31.265
C	-4.160	-2.734	31.964
O	-2.957	-1.986	32.090
C	-4.511	-3.151	33.391
O	-3.777	-4.312	33.767
C	-3.998	-1.972	34.214
C	-2.765	-1.544	33.420
N	-2.534	-0.082	33.414
C	-1.224	0.372	33.427
O	-0.308	-0.450	33.448
N	-0.990	1.711	33.417
C	-2.016	2.568	33.394
N	-1.734	3.872	33.385
C	-3.379	2.132	33.380

C	-3.580	0.796	33.392
H	-0.783	4.187	33.396
H	-2.476	4.541	33.366
H	-5.929	-2.531	30.755
H	-4.719	-1.247	30.532
H	-3.960	-3.617	31.354
H	-5.557	-3.455	33.451
H	-4.766	-1.199	34.257
H	-3.766	-2.305	35.226
H	-1.843	-1.967	33.823
H	-4.179	2.857	33.361
H	-4.594	0.422	33.382
P	2.360	8.887	1.487
O	3.515	9.777	1.229
O	1.118	9.218	0.754
O	2.771	7.369	1.196
C	3.576	6.666	2.161
C	4.411	5.607	1.469
O	3.623	4.387	1.352
C	4.832	5.926	0.034
O	5.974	5.165	-0.347
C	3.639	5.434	-0.785
C	3.191	4.213	0.011
N	1.714	4.015	0.024
C	1.234	2.708	0.018
O	2.046	1.774	0.003
N	-0.108	2.506	0.030
C	-0.953	3.544	0.047
N	-2.254	3.295	0.058
C	-0.481	4.897	0.054
C	0.865	5.076	0.041
H	-2.579	2.363	0.052
H	-2.888	4.029	0.072
H	4.237	7.370	2.666
H	2.928	6.187	2.895
H	5.284	5.375	2.079
H	5.154	6.965	-0.028
H	2.881	6.216	-0.830
H	3.967	5.188	-1.795
H	3.591	3.278	-0.382
H	-1.185	5.715	0.068
H	1.257	6.082	0.045
P	-2.919	9.674	5.216
O	-2.514	11.075	4.964
O	-4.164	9.235	4.547

O	-1.721	8.686	4.830
C	-0.602	8.563	5.728
C	0.650	8.205	4.951
O	0.711	6.757	4.798
C	0.720	8.740	3.521
O	2.066	8.796	3.059
C	-0.012	7.663	2.720
C	0.381	6.392	3.467
N	-0.702	5.371	3.522
C	-2.064	5.551	3.626
N	-2.750	4.434	3.651
C	-1.773	3.444	3.557
C	-1.903	2.031	3.534
O	-2.924	1.351	3.592
N	-0.654	1.404	3.429
C	0.562	2.056	3.355
N	1.640	1.276	3.258
N	0.682	3.382	3.377
C	-0.521	4.006	3.478
H	-0.652	0.424	3.406
H	1.539	0.290	3.242
H	2.505	1.666	3.205
H	-0.444	9.510	6.244
H	-0.806	7.780	6.458
H	1.529	8.511	5.517
H	0.374	9.773	3.501
H	-1.084	7.858	2.744
H	0.337	7.677	1.688
H	1.225	5.875	3.011
H	-2.475	6.549	3.678
P	-7.432	7.055	9.087
O	-7.946	8.431	8.906
O	-8.208	5.986	8.419
O	-5.903	6.983	8.623
C	-4.884	7.517	9.490
C	-3.703	7.997	8.669
O	-2.805	6.873	8.435
C	-4.033	8.517	7.271
O	-3.004	9.375	6.787
C	-4.025	7.243	6.426
C	-2.921	6.429	7.092
N	-3.187	4.963	7.112
C	-2.100	4.104	6.972
O	-0.969	4.589	6.839
N	-2.321	2.765	6.987

C	-3.560	2.280	7.134
N	-3.724	0.966	7.143
C	-4.693	3.146	7.280
C	-4.449	4.481	7.261
H	-2.943	0.370	7.041
H	-4.611	0.588	7.250
H	-5.291	8.355	10.056
H	-4.550	6.742	10.180
H	-3.148	8.745	9.234
H	-4.923	9.144	7.316
H	-5.002	6.764	6.481
H	-3.803	7.496	5.389
H	-1.958	6.528	6.592
H	-5.681	2.727	7.397
H	-5.279	5.164	7.368
P	-9.389	2.217	12.980
O	-10.617	3.038	12.875
O	-9.431	0.908	12.291
O	-8.130	3.058	12.466
C	-7.570	4.072	13.323
C	-6.932	5.164	12.487
O	-5.561	4.779	12.176
C	-7.573	5.418	11.123
O	-7.263	6.723	10.645
C	-6.869	4.402	10.224
C	-5.465	4.373	10.819
N	-4.827	3.027	10.783
C	-5.405	1.785	10.932
N	-4.557	0.789	10.848
C	-3.331	1.415	10.627
C	-2.038	0.857	10.453
O	-1.703	-0.325	10.455
N	-1.073	1.854	10.255
C	-1.324	3.212	10.230
N	-0.265	4.000	10.027
N	-2.537	3.735	10.394
C	-3.485	2.780	10.586
H	-0.148	1.554	10.125
H	0.634	3.600	9.906
H	-0.373	4.943	10.001
H	-8.359	4.505	13.937
H	-6.812	3.625	13.967
H	-6.888	6.086	13.066
H	-8.659	5.407	11.224
H	-7.380	3.442	10.289

H	-6.888	4.754	9.193
H	-4.766	5.024	10.293
H	-6.468	1.701	11.101
P	-7.876	-2.942	16.627
O	-9.354	-3.005	16.608
O	-7.178	-3.999	15.862
O	-7.388	-1.502	16.129
C	-7.484	-0.382	17.030
C	-7.665	0.902	16.244
O	-6.352	1.413	15.871
C	-8.412	0.770	14.917
O	-8.960	2.020	14.510
C	-7.299	0.398	13.938
C	-6.116	1.187	14.489
N	-4.810	0.483	14.354
C	-3.679	1.254	14.100
O	-3.805	2.482	13.999
N	-2.480	0.632	13.973
C	-2.387	-0.699	14.090
N	-1.194	-1.259	13.958
C	-3.538	-1.512	14.351
C	-4.727	-0.869	14.474
H	-0.402	-0.698	13.776
H	-1.098	-2.221	14.039
H	-8.340	-0.520	17.691
H	-6.573	-0.314	17.624
H	-8.139	1.652	16.877
H	-9.273	0.115	15.048
H	-7.140	-0.680	13.959
H	-7.583	0.703	12.931
H	-5.968	2.142	13.984
H	-3.433	-2.583	14.441
H	-5.616	-1.450	14.671
P	-3.118	-6.315	20.451
O	-4.303	-7.216	20.892
O	-2.328	-6.786	19.177
O	-3.761	-4.898	20.085
C	-4.996	-4.441	20.669
C	-5.559	-3.254	19.872
O	-4.475	-2.350	19.690
C	-6.106	-3.656	18.481
O	-7.327	-2.973	18.136
C	-4.942	-3.247	17.588
C	-4.395	-2.035	18.319
N	-3.043	-1.751	17.859

C	-2.043	-2.669	17.831
N	-0.864	-2.154	17.640
C	-1.121	-0.798	17.461
C	-0.210	0.261	17.195
O	1.011	0.207	17.073
N	-0.876	1.472	17.106
C	-2.235	1.664	17.217
N	-2.665	2.915	17.096
N	-3.085	0.665	17.475
C	-2.465	-0.534	17.568
H	-0.318	2.287	16.911
H	-2.035	3.669	16.900
H	-3.638	3.124	17.167
H	-5.754	-5.224	20.674
H	-4.803	-4.133	21.697
H	-6.354	-2.783	20.454
H	-6.276	-4.731	18.412
H	-4.266	-4.098	17.590
H	-5.153	-2.992	16.555
H	-4.961	-1.147	18.168
H	-2.281	-3.702	18.030
P	2.557	-6.607	26.063
O	2.062	-8.015	26.489
O	3.808	-6.496	25.151
O	1.313	-5.882	25.305
C	0.927	-6.163	23.924
C	-0.529	-5.700	23.622
O	-0.787	-4.542	24.416
C	-0.953	-5.429	22.136
O	-2.232	-6.107	21.855
C	-0.963	-3.882	22.154
C	-1.022	-3.392	23.625
N	-0.027	-2.295	23.946
C	-0.417	-0.963	23.823
O	-1.613	-0.672	23.845
N	0.519	0.003	23.606
C	1.820	-0.322	23.564
N	2.698	0.654	23.360
C	2.268	-1.663	23.770
C	1.309	-2.589	23.985
H	2.405	1.598	23.210
H	3.678	0.440	23.318
H	1.625	-5.673	23.245
H	0.981	-7.238	23.741
H	-1.172	-6.488	24.016

H	-0.194	-5.805	21.449
H	-0.038	-3.534	21.693
H	-1.804	-3.486	21.582
H	-2.043	-3.076	23.843
H	3.325	-1.893	23.728
H	1.614	-3.615	24.118
P	7.465	-3.173	28.870
O	8.004	-4.607	28.770
O	8.168	-2.184	27.928
O	5.897	-3.163	28.577
C	5.017	-3.582	29.623
C	3.736	-4.155	29.018
O	2.834	-3.084	28.761
C	3.910	-4.855	27.662
O	2.837	-5.765	27.442
C	3.776	-3.688	26.690
C	2.750	-2.796	27.379
N	3.000	-1.350	27.181
C	4.192	-0.674	27.073
N	4.061	0.613	26.908
C	2.684	0.814	26.882
C	1.931	2.008	26.727
O	2.342	3.151	26.558
N	0.569	1.745	26.758
C	-0.013	0.510	26.951
N	-1.344	0.487	26.936
N	0.699	-0.614	27.080
C	2.031	-0.380	27.050
H	-0.045	2.535	26.665
H	-1.879	1.328	26.838
H	-1.825	-0.375	27.077
H	5.503	-4.341	30.237
H	4.763	-2.725	30.248
H	3.281	-4.826	29.751
H	4.806	-5.474	27.689
H	4.747	-3.219	26.551
H	3.433	-4.062	25.724
H	1.735	-2.963	27.019
H	5.127	-1.212	27.145
P	9.760	2.165	31.745
O	11.044	1.331	31.575
O	9.698	3.404	30.830
O	8.477	1.244	31.506
C	8.073	0.374	32.562
C	7.343	-0.833	31.979

O	5.969	-0.513	31.797
C	7.829	-1.274	30.599
O	7.488	-2.636	30.360
C	6.988	-0.410	29.664
C	5.670	-0.301	30.430
N	4.997	1.009	30.282
C	3.612	1.031	30.246
O	3.006	-0.038	30.316
N	2.974	2.223	30.115
C	3.682	3.354	30.025
N	3.009	4.498	29.898
C	5.113	3.365	30.059
C	5.719	2.165	30.189
H	2.008	4.500	29.871
H	3.507	5.362	29.829
H	8.944	0.038	33.125
H	7.391	0.901	33.231
H	7.417	-1.662	32.686
H	8.918	-1.244	30.553
H	7.479	0.553	29.523
H	6.886	-0.904	28.698
H	4.931	-1.031	30.095
H	5.649	4.300	29.984
H	6.799	2.128	30.219
P	8.698	7.766	34.868
O	10.216	7.841	34.610
O	7.876	8.765	34.031
O	8.176	6.278	34.610
C	8.414	5.302	35.623
C	8.488	3.916	34.991
O	7.176	3.381	34.867
C	9.059	3.884	33.574
O	9.566	2.589	33.272
C	7.819	4.126	32.716
C	6.730	3.423	33.525
N	5.415	4.105	33.475
C	5.130	5.448	33.428
N	3.855	5.726	33.397
C	3.242	4.476	33.425
C	1.865	4.130	33.412
O	0.885	4.872	33.370
N	1.694	2.752	33.452
C	2.705	1.817	33.500
N	2.315	0.542	33.532
N	4.001	2.140	33.513

C	4.187	3.483	33.473
H	0.749	2.411	33.446
H	1.344	0.294	33.523
H	2.999	-0.181	33.569
H	9.349	5.519	36.141
H	7.594	5.312	36.342
H	9.069	3.263	35.645
H	9.923	4.544	33.498
H	7.651	5.198	32.619
H	7.969	3.693	31.727
H	6.533	2.411	33.168
H	5.935	6.171	33.419
O	-6.421	-6.784	-2.970
H	-6.364	-5.835	-3.102
P	-3.541	-4.599	35.322
O	-3.621	-6.120	35.557
O	-4.526	-3.787	36.186
O	-2.050	-4.087	35.574
H	-1.817	-4.221	36.495
P	6.296	4.986	-1.901
O	7.756	5.022	-2.141
O	5.493	5.958	-2.676
O	5.741	3.507	-2.150
H	4.794	3.489	-1.993
O	8.360	7.928	36.422
H	7.407	7.888	36.529