

Supporting Information

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Cytotoxic sesterterpenoids from Bornean sponge *Spongia* sp.

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Korimoto, Kagoshima 890-0065, Japan*

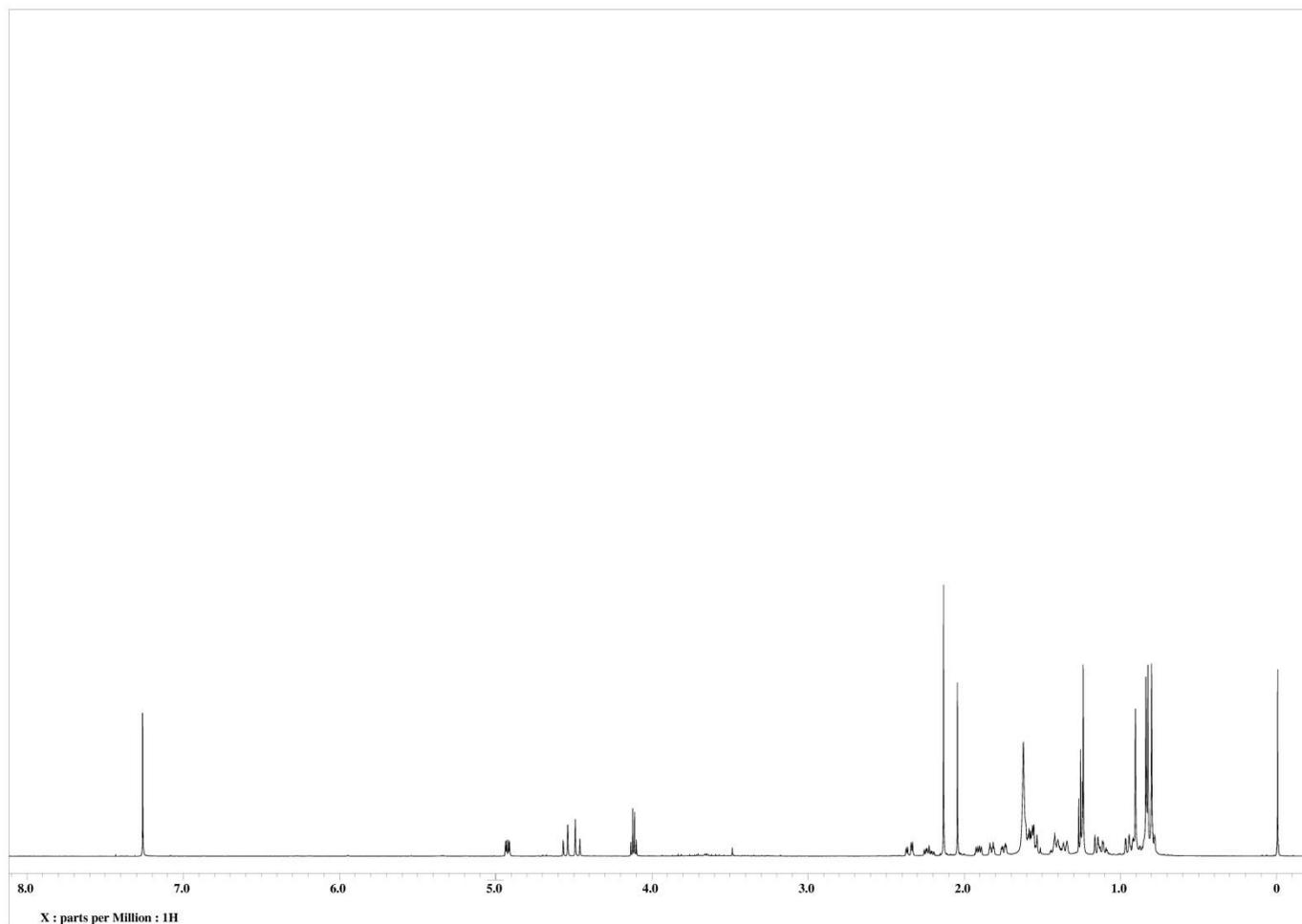
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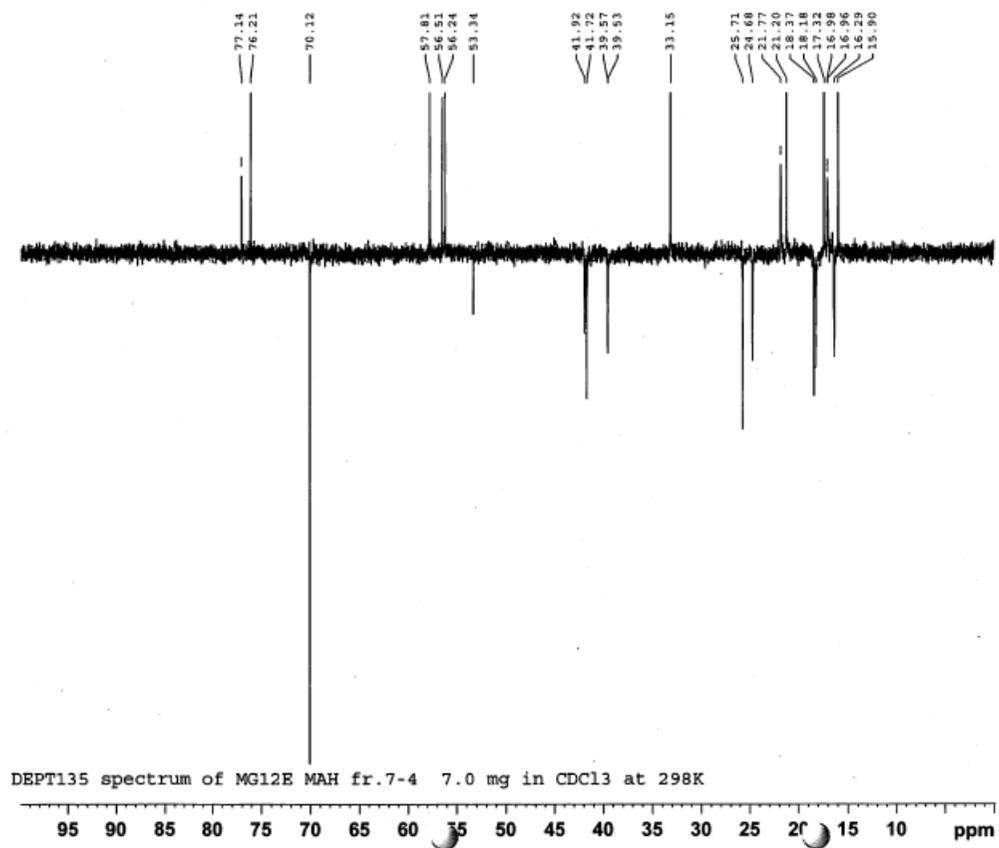
Table S1: ^{13}C and ^1H NMR data of **1-4** (CDCl_3 , δ in ppm).

No	1		2		3		4	
	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}
1	39.5	1.62-1.65 m	39.9	1.72-1.75 m	39.9	1.70-1.71 m	39.7	1.73-1.75 m
		0.83-0.85 m		0.78-0.80 m		0.79-0.80 m		0.80-0.81 m
2	18.4	1.58-1.60 m	18.7	1.60-1.62 m	18.5	1.60-1.62 m	18.4	1.60-1.61 m
		1.40-1.42 m		1.40-1.42 m		1.42-1.44 m		1.42-1.44 m
3	41.9	1.35 m	42.4	1.37 m	42.0	1.36-1.38 m	42.0	1.36-1.38 m
		1.11 m		1.12 m		1.13 td (13.3, 4.1)		1.12-1.13 m
4	33.1		33.5		33.2		33.1	
5	56.5	0.80-0.81 m	57.0	0.77-0.78 m	56.4	0.79-0.80 m	56.4	0.79-0.80 m
6	18.2	1.58-1.60 m	18.4	1.57-1.59 m	18.0	1.53-1.55 m	17.9	1.52-1.54 m
		1.40-1.42 m		1.40-1.42 m		1.36-1.38 m		1.36-1.38 m
7	41.7	1.82 dt (12.2, 3.4)	42.0	1.83 m	41.4	1.69-1.71 m	41.0	1.67-1.69 m
		0.92-0.94 m		0.90-0.92 m		0.90-0.92 m		0.87-0.88 m
8	37.3		37.3		37.3		37.3	
9	57.8	0.95-0.96 m	58.1	0.87-0.88 m	58.8	0.89-0.91 m	57.9	0.87-0.88 m
10	37.2		37.5		37.3		37.3	
11	24.7	1.75 ddd (12.9, 4.8, 2.7)	25.9	1.86 m	26.0	1.75-1.76 m	25.2	1.76-1.77 m
		1.55-1.57 m		1.50-1.52 m		1.44-1.46 m		1.42-1.44 m
12	76.2	4.92 dd (10.9, 4.8)	76.0	3.66 dd (11.0, 4.6)	80.2	3.51 dt (11.5, 3.7)	81.6	3.67 dd (11.5, 4.6)

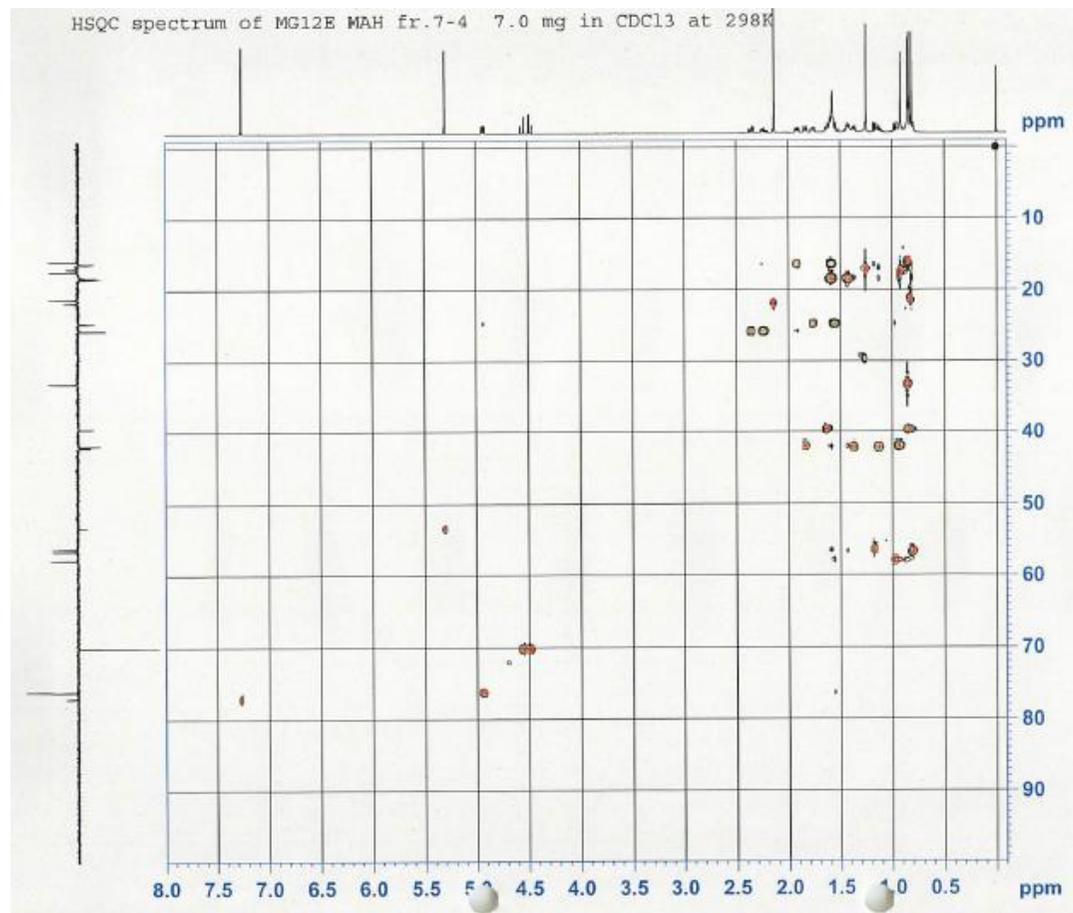
13	41.1		42.5		39.9		41.2	
14	56.2	1.15 d (11.6)	55.5	1.17 m	52.7	1.18-1.20 m	50.6	1.12-1.13 m
15	16.3	1.91 dd (13.6, 6.8)	16.5	1.93 m	23.6	2.34 ddt (20.6, 5.5, 4.1)	23.6	2.18-2.20 m
		1.58-1.60 m		1.64-1.66 m		2.14 dddd (20.6, 11.5, 5.0, 4.1)		
16	25.7	2.35 dd (18.4, 5.4)	25.5	2.44 dd (18.8, 5.5)	136.3	6.86 br m	141.8	6.99 br m
		2.22 ddd (18.4, 11.6, 6.8)		2.26 ddd (18.8, 11.5, 7.3)				
17	161.3		163.0		127.0		129.0	
18	134.4		136.0		57.0	2.52-2.54 m	79.0	4.37 s
19	171.0		176.0		105.5	5.34 d (6.4)	-	
20	70.1	4.55 d (17.0)	72.3	4.72 d (17.4)	167.0		168.0	
		4.47 d (17.0)		4.66 d (17.4)				
21	33.1	0.84 s	33.5	0.85 s	33.2	0.84 s	33.1	0.83 s
22	21.2	0.80 s	21.5	0.81 s	21.3	0.80 s	21.2	0.80 s
23	15.9	0.82 s	16.0	0.84 s	16.5	0.86 s	16.4	0.86 s
24	17.3	0.90 s	17.4	0.89 s	16.7	0.92 s	16.5	0.93 s
25	17.0	1.24 s	16.9	1.12 s	9.1	0.81 s	7.2	0.90 s
OAc	171.5							
	21.8	2.13 s						
OMe					57.9	3.62 s	51.7	3.76 s
OH				5.93 s				4.07 s
OH								4.74 s



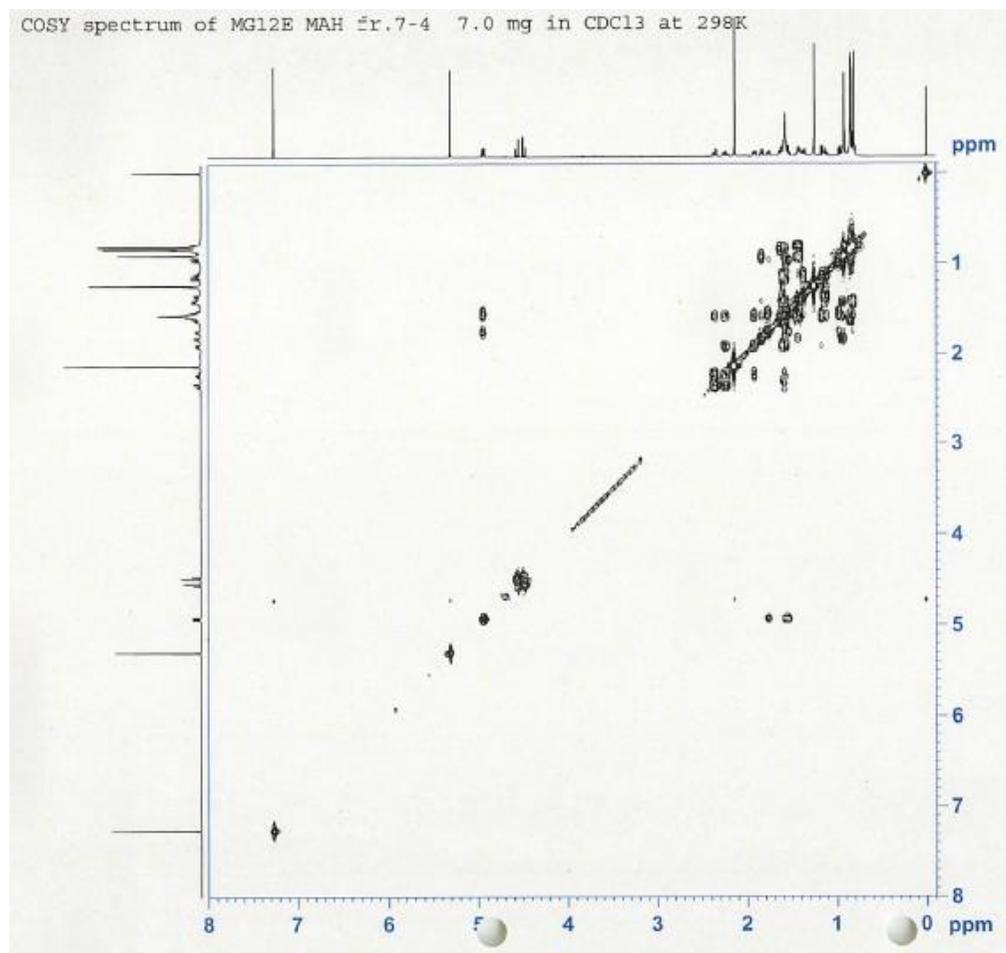
S1: ^1H NMR spectrum of **1** in CDCl_3 .



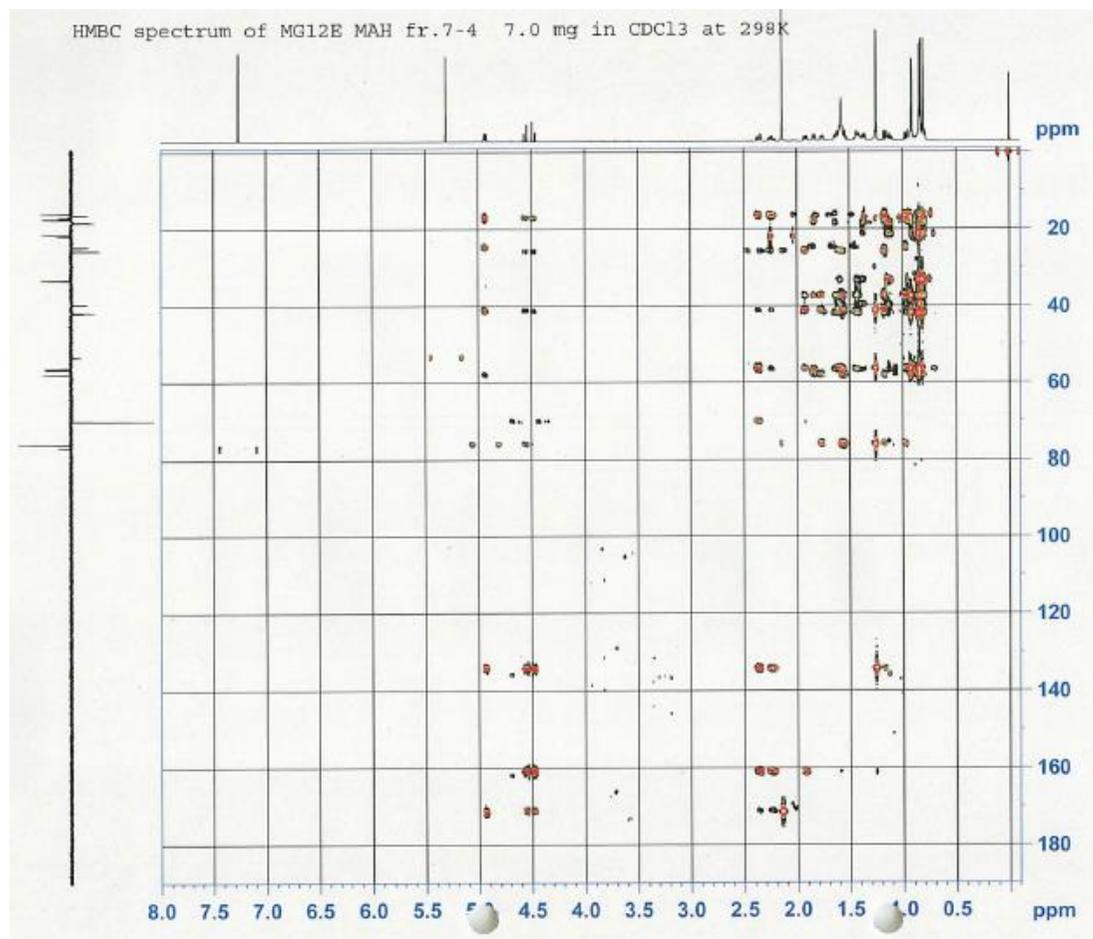
S2: DEPT-135 spectrum of **1** in CDCl₃.



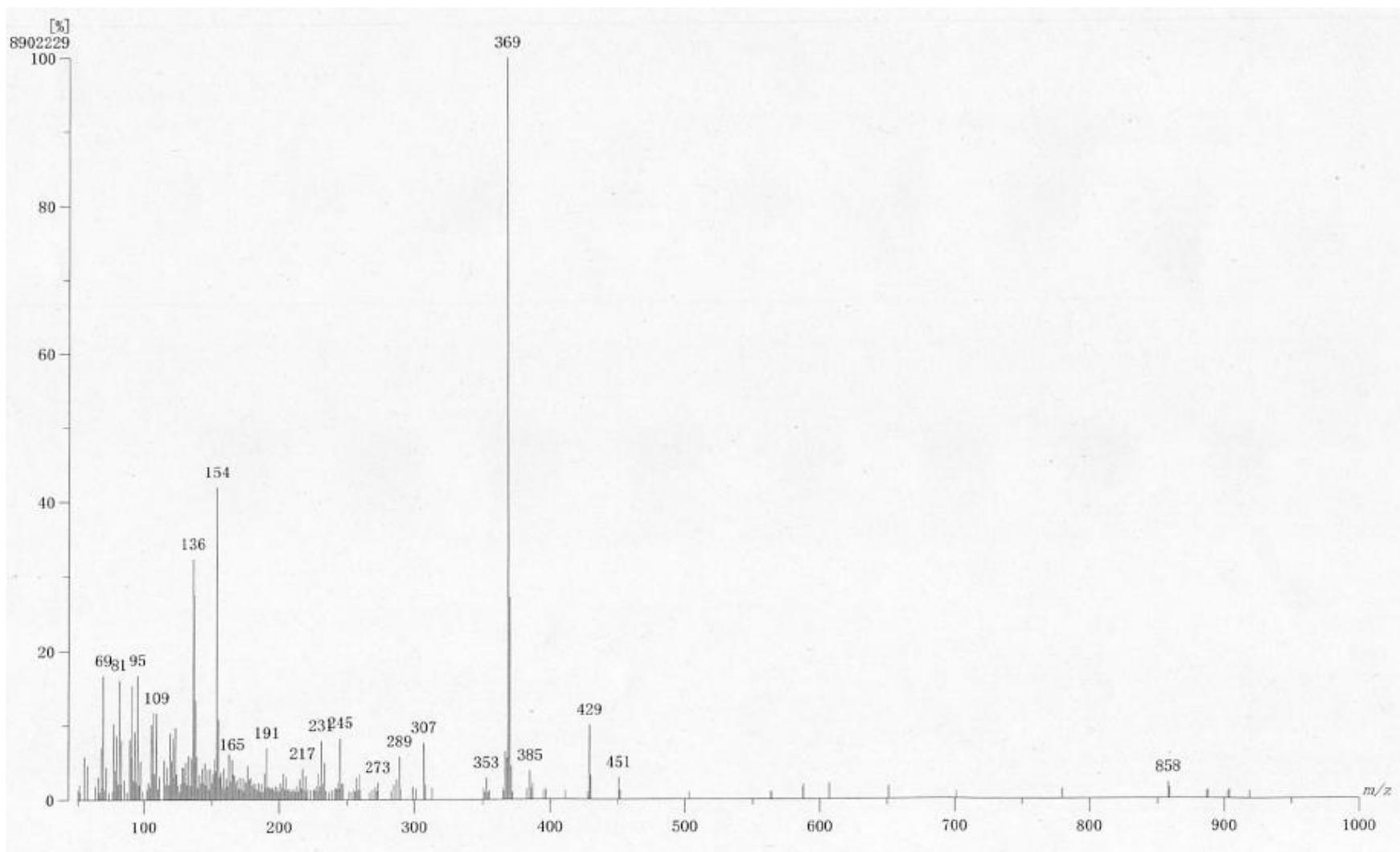
S3: HSQC spectrum of 1 in CDCl₃.



S4: ^1H - ^1H COSY spectrum of **1** in CDCl_3 .

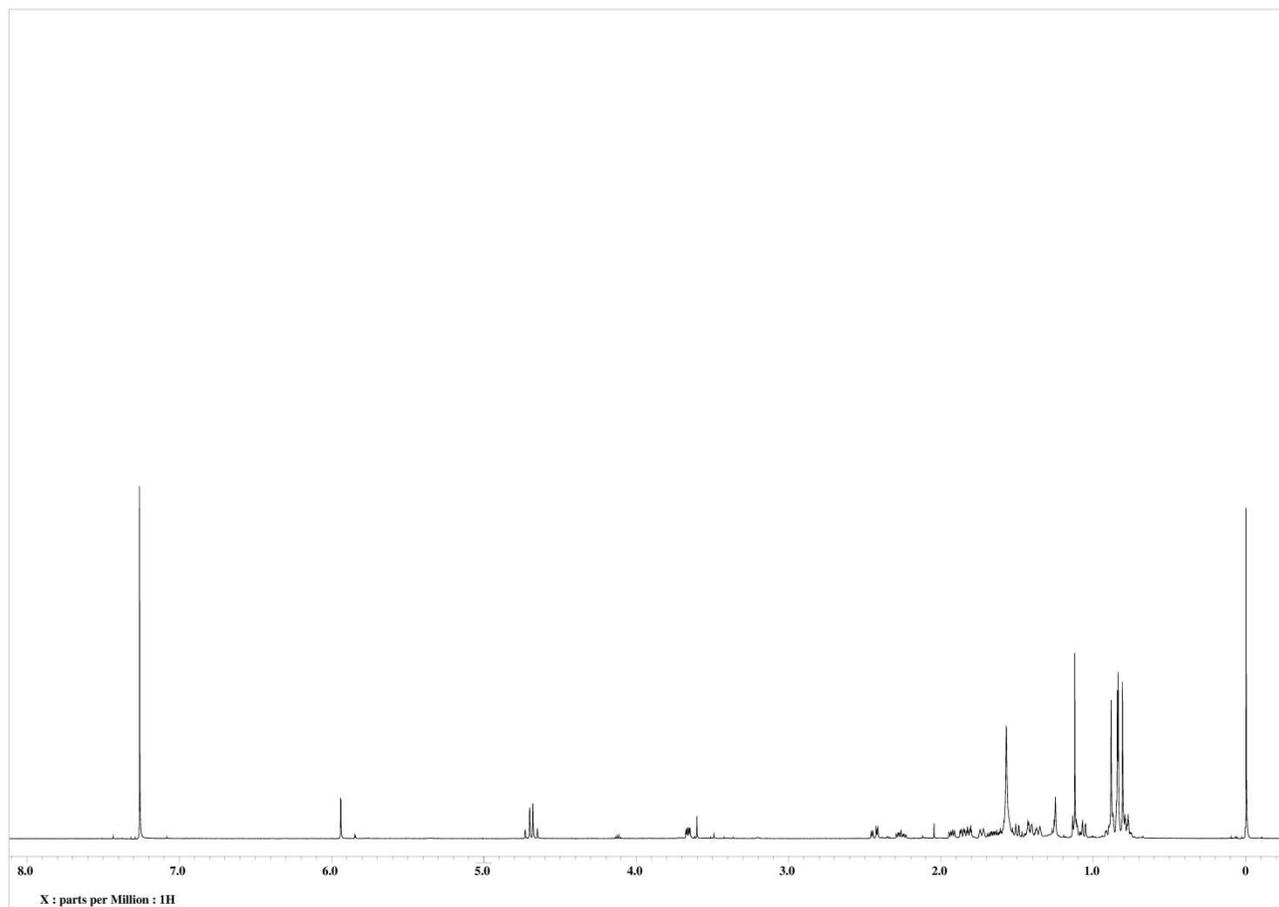


S5: HMBC spectrum of **1** in CDCl₃.

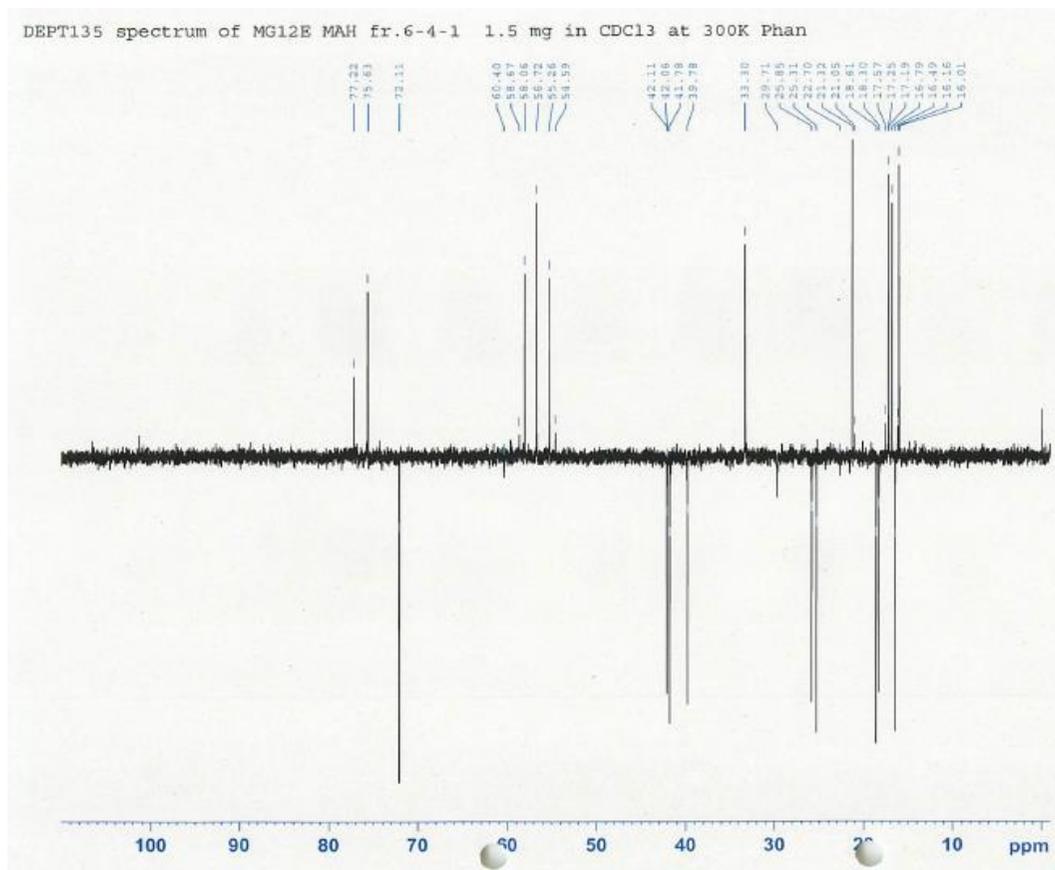


S6: FABMS spectrum of **1**.

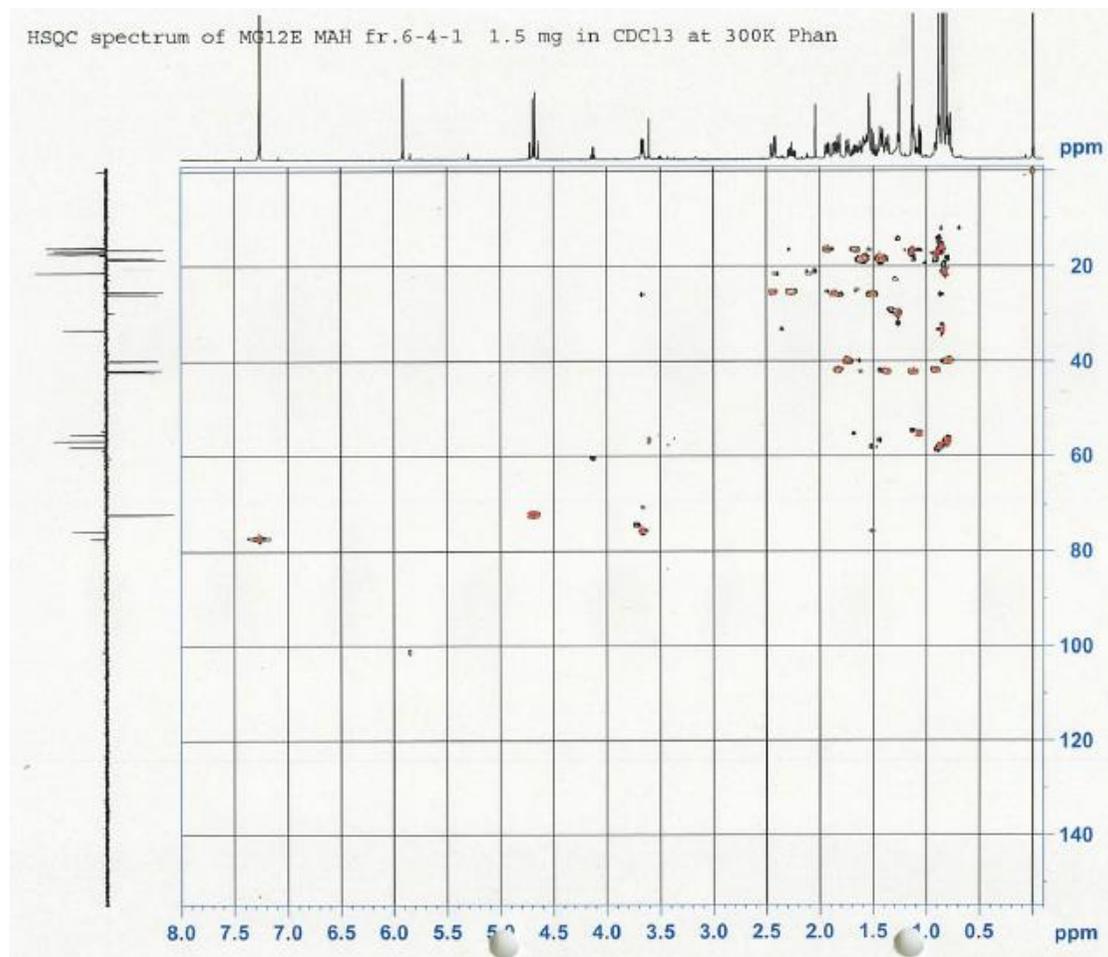
m/z	Int.	Norm.	
301	12.61	1.49	132266
307	65.36	7.70	685376
308	16.97	2.00	177962
313	13.27	1.56	139114
351	13.58	1.60	142442
352	9.33	1.10	97877
353	24.76	2.92	259626
354	8.79	1.04	92202
355	10.89	1.28	114176
365	13.82	1.63	144896
366	10.18	1.20	106794
367	55.50	6.54	581909
368	48.25	5.68	505941
369	848.98	100.00	8902229
370	231.36	27.25	2425941
371	38.96	4.59	408554
372	9.13	1.08	95765
383	12.42	1.46	130261
385	33.34	3.93	349610
386	13.78	1.62	144512
387	18.95	2.23	198656
395	10.48	1.23	109888
397	12.63	1.49	132416
411	10.24	1.21	107392
428	9.17	1.08	96106
429	85.49	10.07	896426
430	28.22	3.32	295957
451	25.03	2.95	262506
452	10.48	1.23	109930
503	8.86	1.04	92906
563	9.39	1.11	98453
564	8.78	1.03	92032
587	13.55	1.60	142037
588	17.33	2.04	181696
607	19.18	2.26	201066
651	15.18	1.79	159168
701	9.05	1.07	94890
780	11.77	1.39	123456
858	19.44	2.29	203818
859	13.02	1.53	136576
887	9.88	1.16	103552
888	10.01	1.18	104981
903	8.78	1.03	92032
904	10.94	1.29	114752
919	9.11	1.07	95552



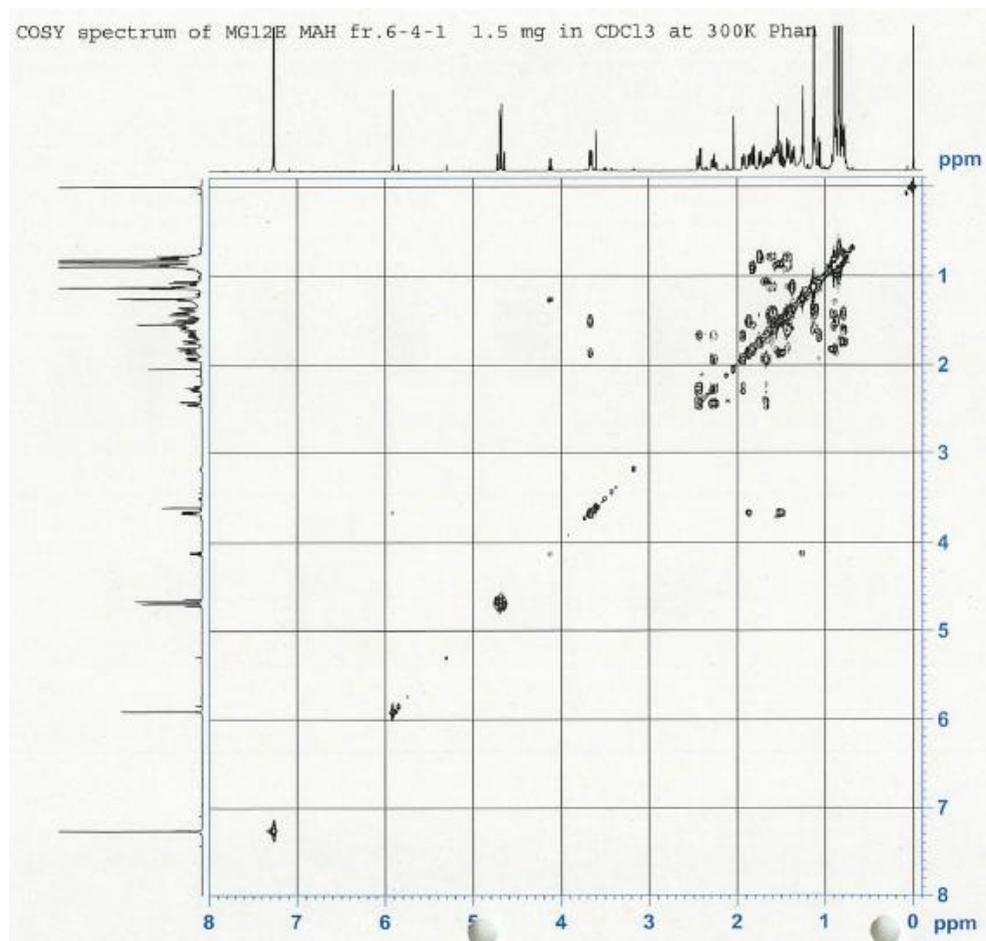
S7: ^1H NMR spectrum of **2** in CDCl_3 .



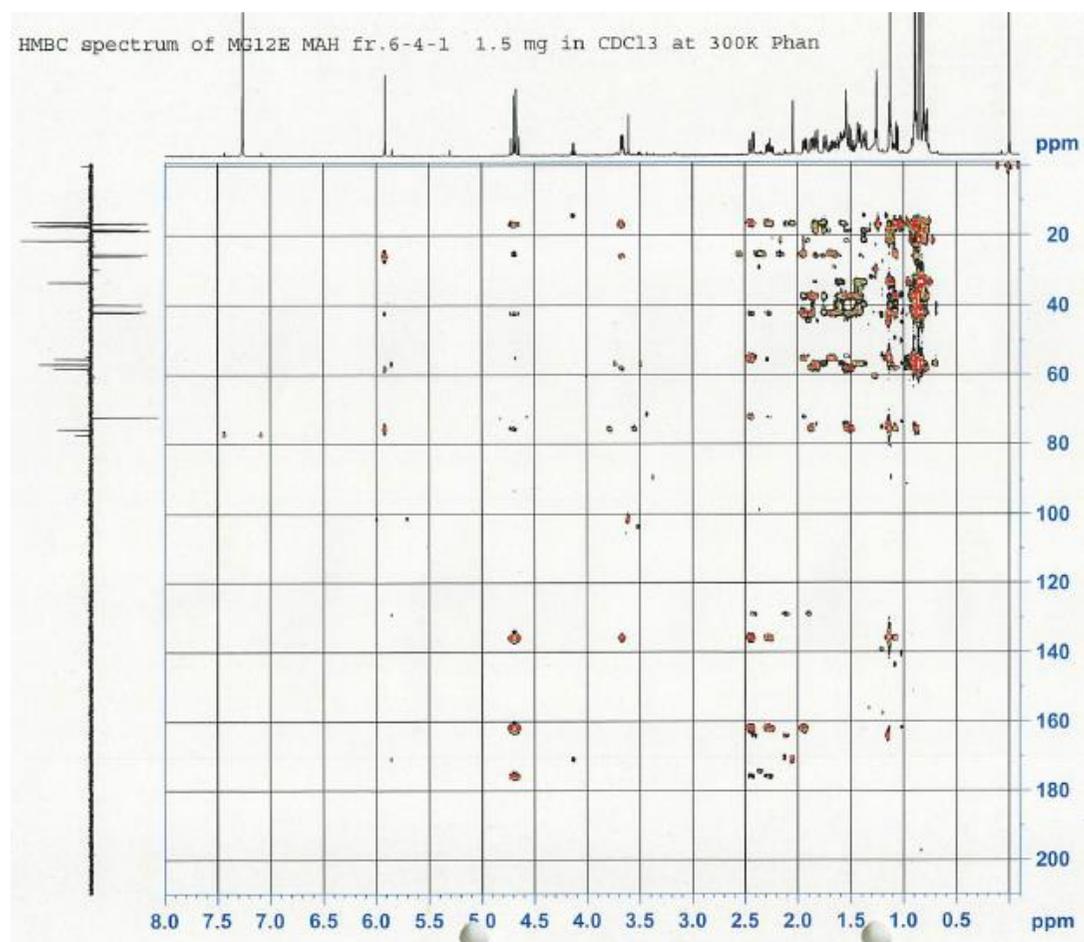
S8: DEPT-135 spectrum of **2** in CDCl₃.



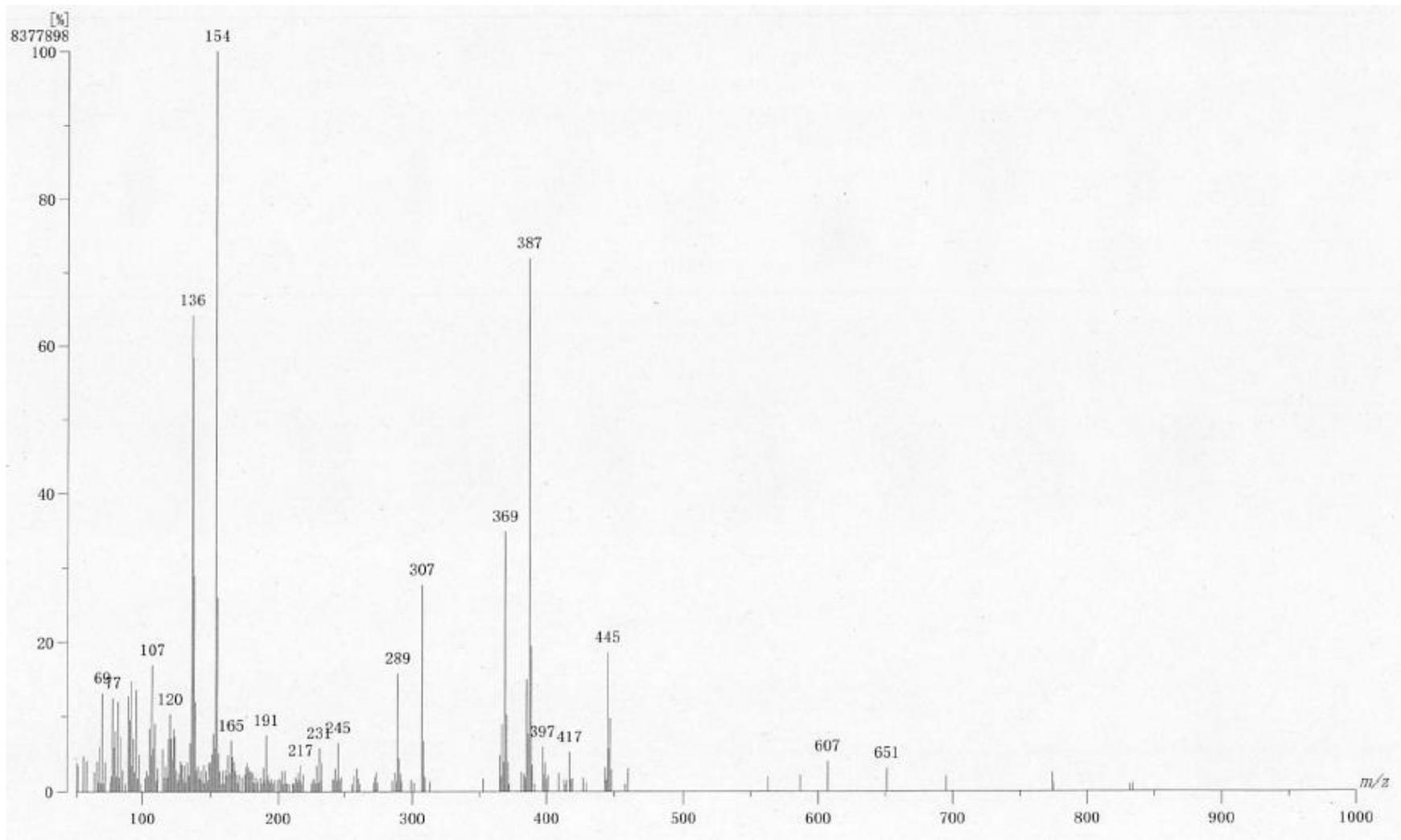
S9: HSQC spectrum of **2** in CDCl₃.



S10: ^1H - ^1H COSY spectrum of **2** in CDCl_3 .



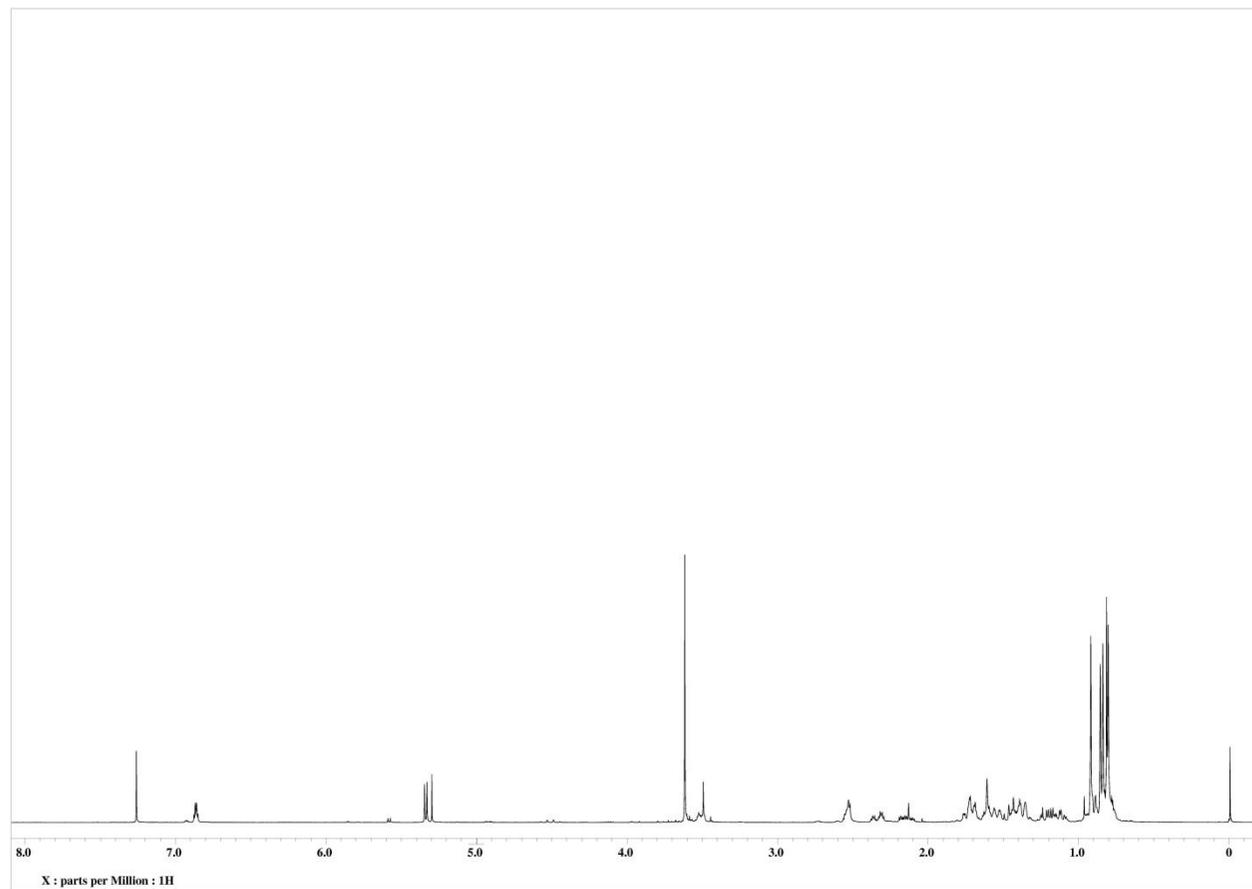
S11: HMBC spectrum of **2** in CDCl₃.



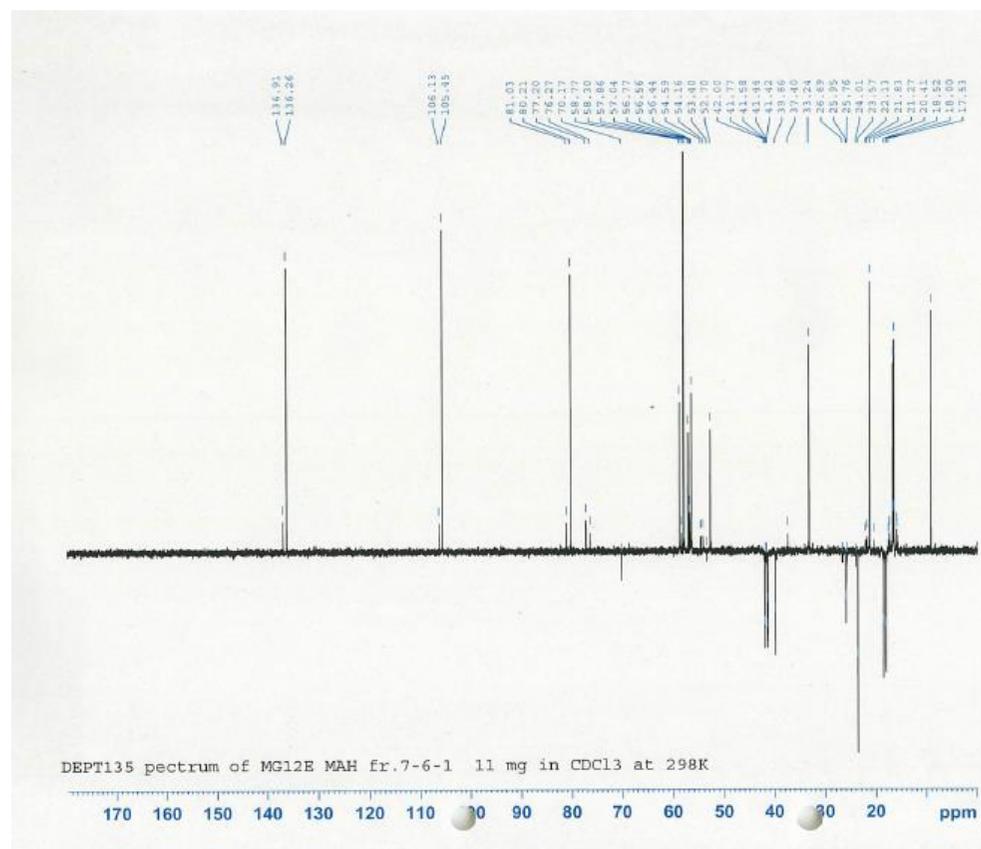
S12: FABMS spectrum of 2.

m/z	Int.	Norm.	
201	12.96	1.62	135893
202	11.67	1.46	122346
203	20.87	2.61	218794
204	8.31	1.04	87104
205	20.90	2.62	219200
206	9.58	1.20	100501
207	8.36	1.05	87637
209	8.31	1.04	87125
211	9.18	1.15	96234
212	8.74	1.09	91648
213	14.27	1.79	149653
214	10.94	1.37	114752
215	19.00	2.38	199189
216	11.75	1.47	123200
217	26.84	3.36	281450
218	10.05	1.26	105386
219	16.91	2.12	177322
225	8.40	1.05	88128
226	10.91	1.37	114368
227	12.93	1.62	135594
228	9.46	1.18	99178
229	26.81	3.36	281109
230	10.34	1.29	108373
231	45.63	5.71	478506
232	11.38	1.42	119338
233	29.87	3.74	313258
241	12.12	1.52	127125
242	12.06	1.51	126421
243	23.34	2.92	244714
244	11.49	1.44	120469
245	51.23	6.41	537237
246	12.02	1.50	126037
247	13.92	1.74	145941
255	8.15	1.02	85418
257	15.83	1.98	165994
259	23.57	2.95	247104
260	13.16	1.65	137984
261	8.43	1.05	88384
271	9.47	1.19	99285
272	14.12	1.77	148032
273	19.31	2.42	202517
274	9.47	1.19	99349
285	11.00	1.38	115349
287	18.66	2.34	195712
288	10.66	1.33	111786
289	126.14	15.79	1322624

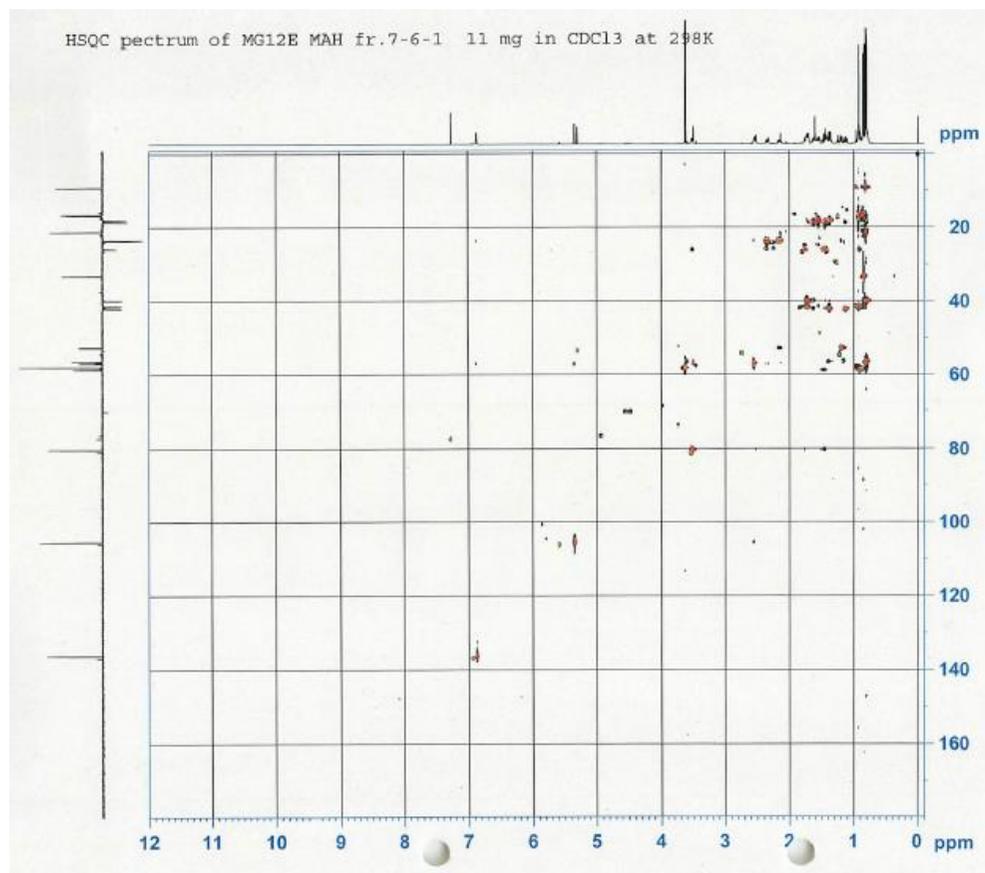
292	10.82	1.35	113429
299	11.38	1.42	119317
301	9.69	1.21	101610
307	221.18	27.68	2319274
308	52.97	6.63	555456
309	14.16	1.77	148437
313	10.61	1.33	111253
353	12.78	1.60	134016
365	37.83	4.73	396650
366	15.18	1.90	159210
367	71.66	8.97	751360
368	30.55	3.82	320362
369	278.50	34.86	2920320
370	81.87	10.25	858496
371	30.70	3.84	321898
372	8.29	1.04	86954
381	19.70	2.47	206549
383	17.52	2.19	183680
384	13.54	1.70	142016
385	119.79	14.99	1256064
386	61.23	7.66	642069
387	575.21	71.99	6031488
388	155.71	19.49	1632768
389	27.67	3.46	290090
391	8.14	1.02	85333
397	47.03	5.89	493120
398	17.16	2.15	179904
399	29.58	3.70	310186
400	12.56	1.57	131690
401	15.96	2.00	167402
409	17.85	2.23	187221
413	11.30	1.41	118442
414	8.08	1.01	84693
415	11.00	1.38	115392
417	41.16	5.15	431552
418	12.09	1.51	126784
419	12.82	1.60	134464
427	13.22	1.65	138645
429	9.86	1.23	103381
443	24.66	3.09	258602
444	11.34	1.42	118954
445	148.74	18.62	1559680
446	45.57	5.70	477845
447	77.93	9.75	817109
448	22.80	2.85	239082
458	8.11	1.01	85013
460	23.71	2.97	248640
563	14.60	1.83	153109
587	16.19	2.03	169770
607	31.64	3.96	331818
651	23.97	3.00	251392
695	14.90	1.86	156224
774	19.06	2.39	199829
775	9.41	1.18	98688
832	8.15	1.02	85504
834	9.00	1.13	94400



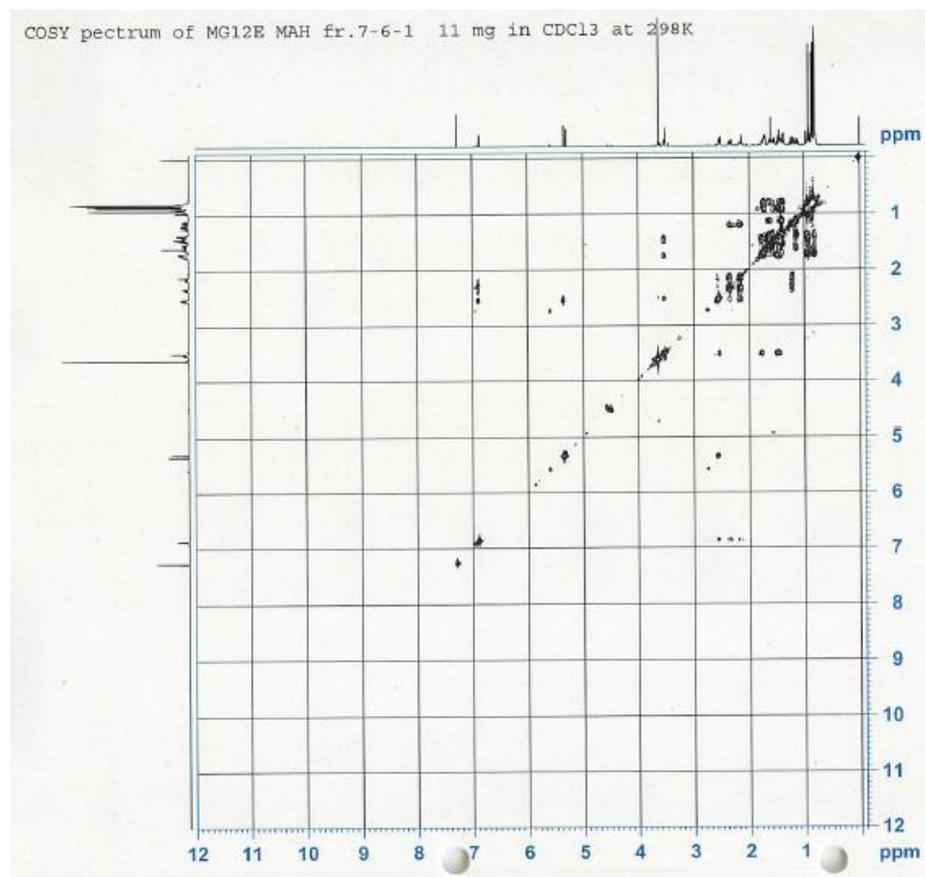
S13: ^1H NMR spectrum of **3** in CDCl_3 .



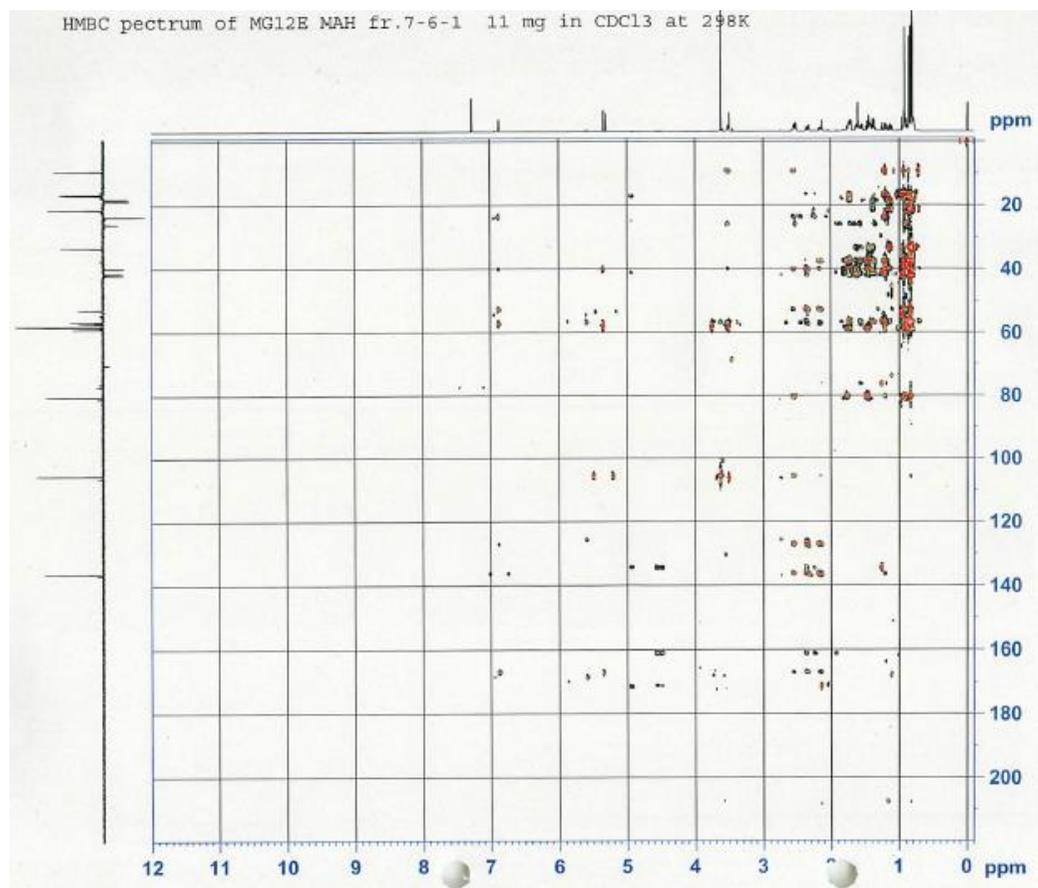
S14: DEPT-135 spectrum of **3** in CDCl₃.



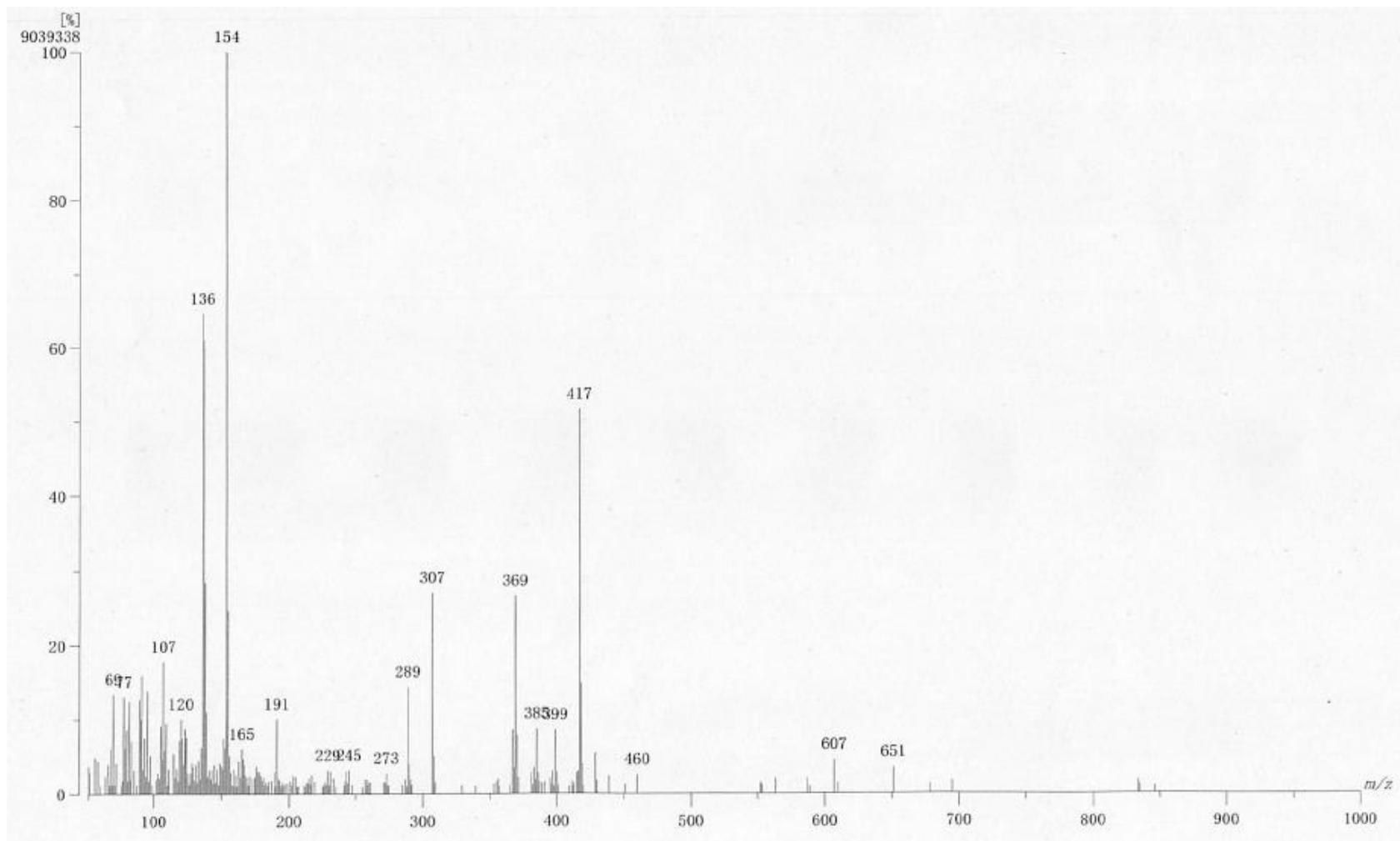
S15: HSQC spectrum of **3** in CDCl₃.



S16: ^1H - ^1H COSY spectrum of **3** in CDCl_3 .



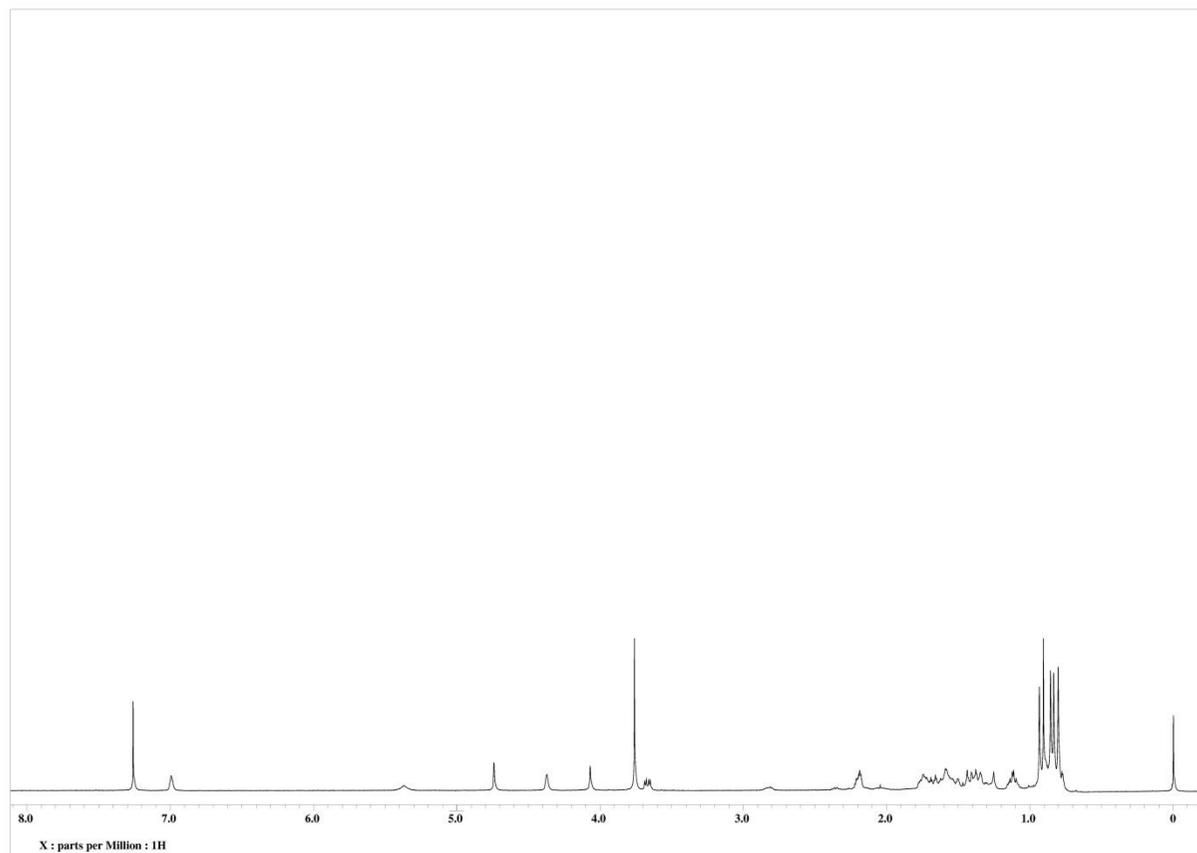
S17: HMBC spectrum of **3** in CDCl₃.



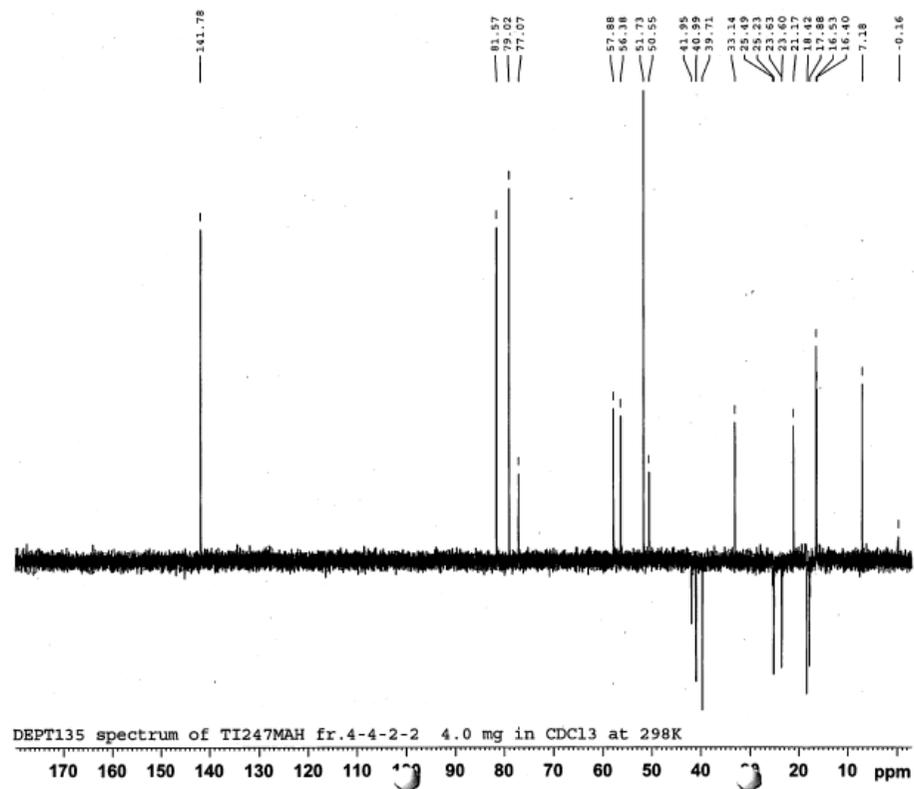
S18: FABMS spectrum of **3**.

m/z	Int.	Norm.	
255	8.77	1.02	91968
257	16.36	1.90	171562
258	10.34	1.20	108373
259	16.36	1.90	171498
260	13.03	1.51	136597
261	14.11	1.64	147968
271	13.64	1.58	143061
272	13.15	1.53	137856
273	23.85	2.77	250133
274	11.12	1.29	116650
275	10.14	1.18	106346
285	10.88	1.26	114048
287	17.02	1.97	178517
288	9.41	1.09	98709
289	124.30	14.42	1303360
290	34.82	4.04	365098
291	16.80	1.95	176192
292	11.03	1.28	115690
307	233.08	27.04	2444010
308	43.91	5.09	460394
309	13.68	1.59	143488
329	10.23	1.19	107285
339	9.35	1.08	98005
353	11.39	1.32	119402
355	13.95	1.62	146261
356	18.09	2.10	189653
357	9.13	1.06	95786
365	10.24	1.19	107328
367	74.97	8.70	786112
368	30.81	3.57	323072
369	229.40	26.61	2405440
370	68.70	7.97	720405
371	19.77	2.29	207338
381	24.41	2.83	255936
382	10.42	1.21	109226
383	30.95	3.59	324501
384	16.51	1.91	173077
385	76.16	8.83	798613
386	24.24	2.81	254165
387	13.80	1.60	144661
389	12.69	1.47	133056
391	13.40	1.55	140480
395	18.66	2.16	195648
396	11.70	1.36	122730
397	26.66	3.09	279594
398	9.19	1.07	96405

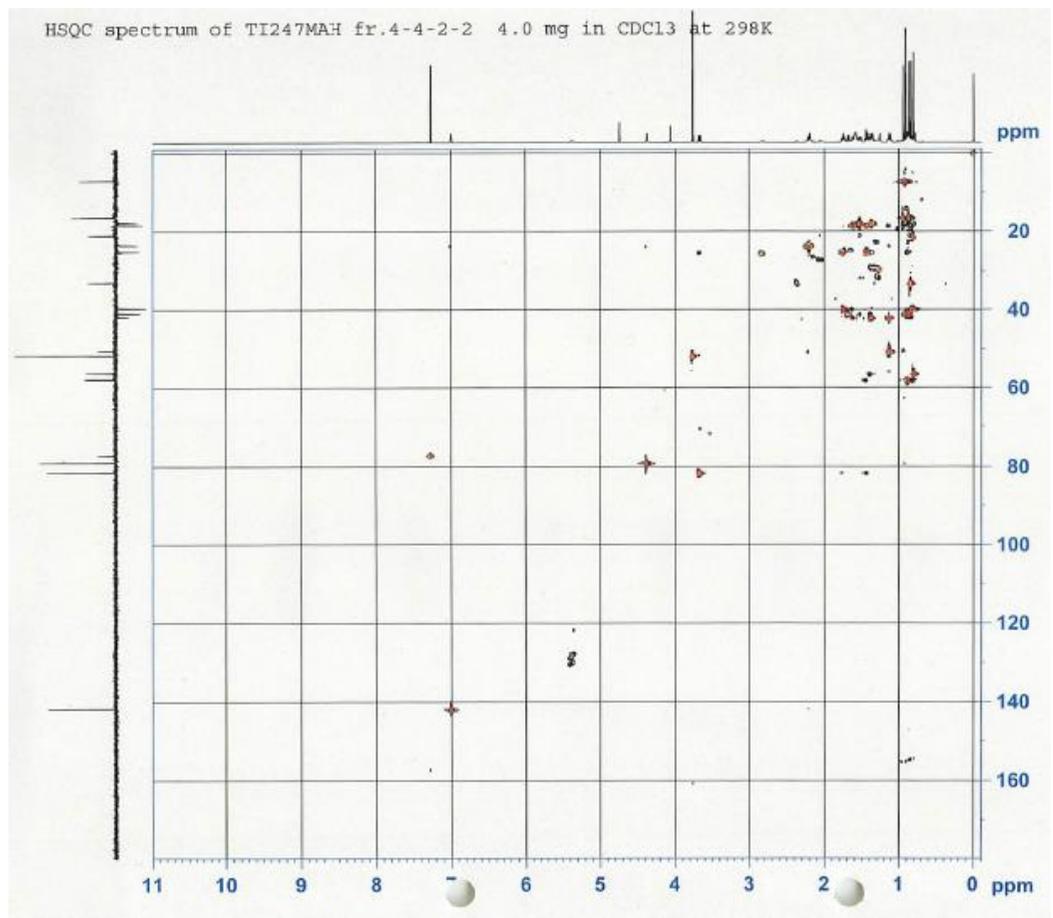
399	74.68	8.66	783040
400	25.84	3.00	270997
401	10.20	1.18	106986
409	8.69	1.01	91136
411	15.23	1.77	159658
412	9.28	1.08	97344
413	12.72	1.48	133333
415	24.90	2.89	261077
416	26.87	3.12	281770
417	444.91	51.61	4665194
418	128.46	14.90	1347050
419	35.21	4.08	369216
420	9.65	1.12	101141
429	47.80	5.54	501184
430	15.54	1.80	162986
439	20.93	2.43	219498
451	11.08	1.29	116160
460	22.43	2.60	235200
552	12.83	1.49	134570
553	10.61	1.23	111253
563	18.43	2.14	193301
587	18.52	2.15	194197
589	9.03	1.05	94677
607	39.78	4.61	417152
610	12.35	1.43	129493
651	30.93	3.59	324352
678	11.47	1.33	120234
695	14.98	1.74	157056
834	16.02	1.86	167936
835	10.18	1.18	106709
846	8.76	1.02	91882



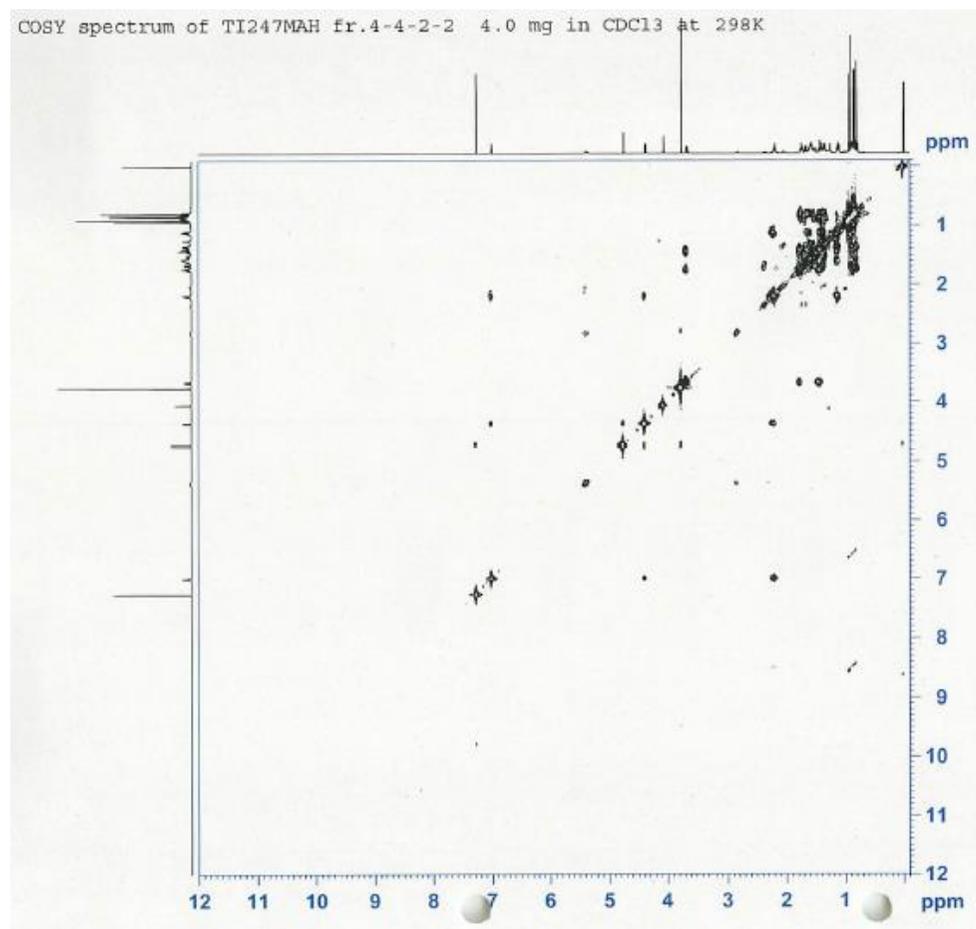
S19: ^1H NMR spectrum of **4** in CDCl_3 .



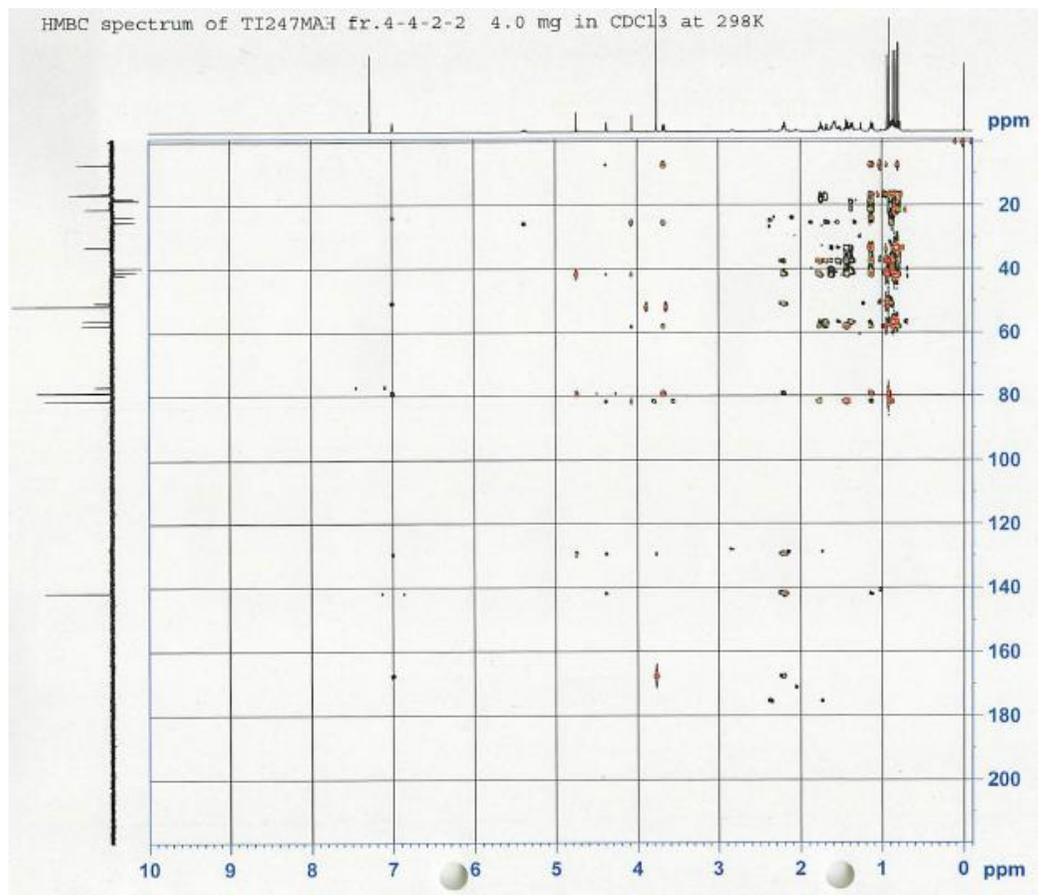
S20: DEPT-135 spectrum of **4** in CDCl₃.



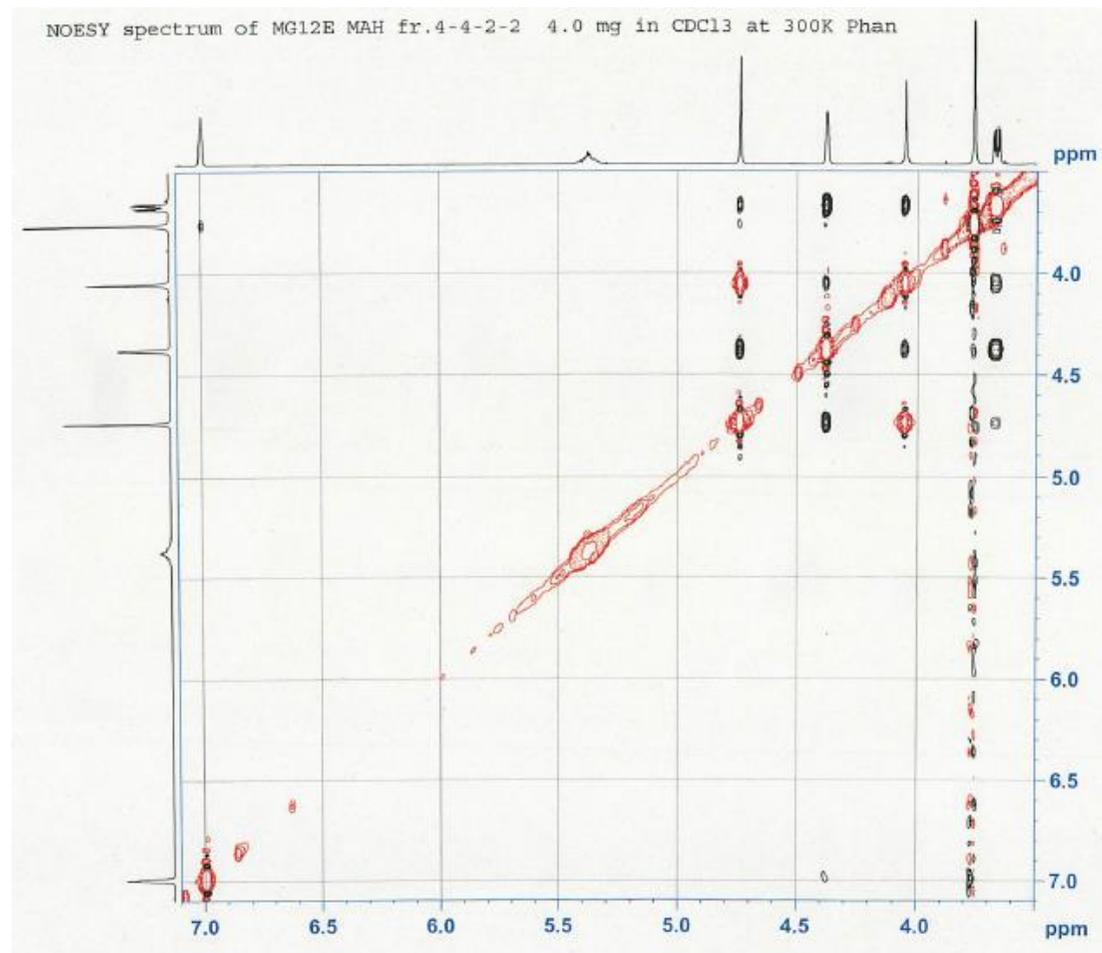
S21: HSQC spectrum of **4** in CDCl₃.



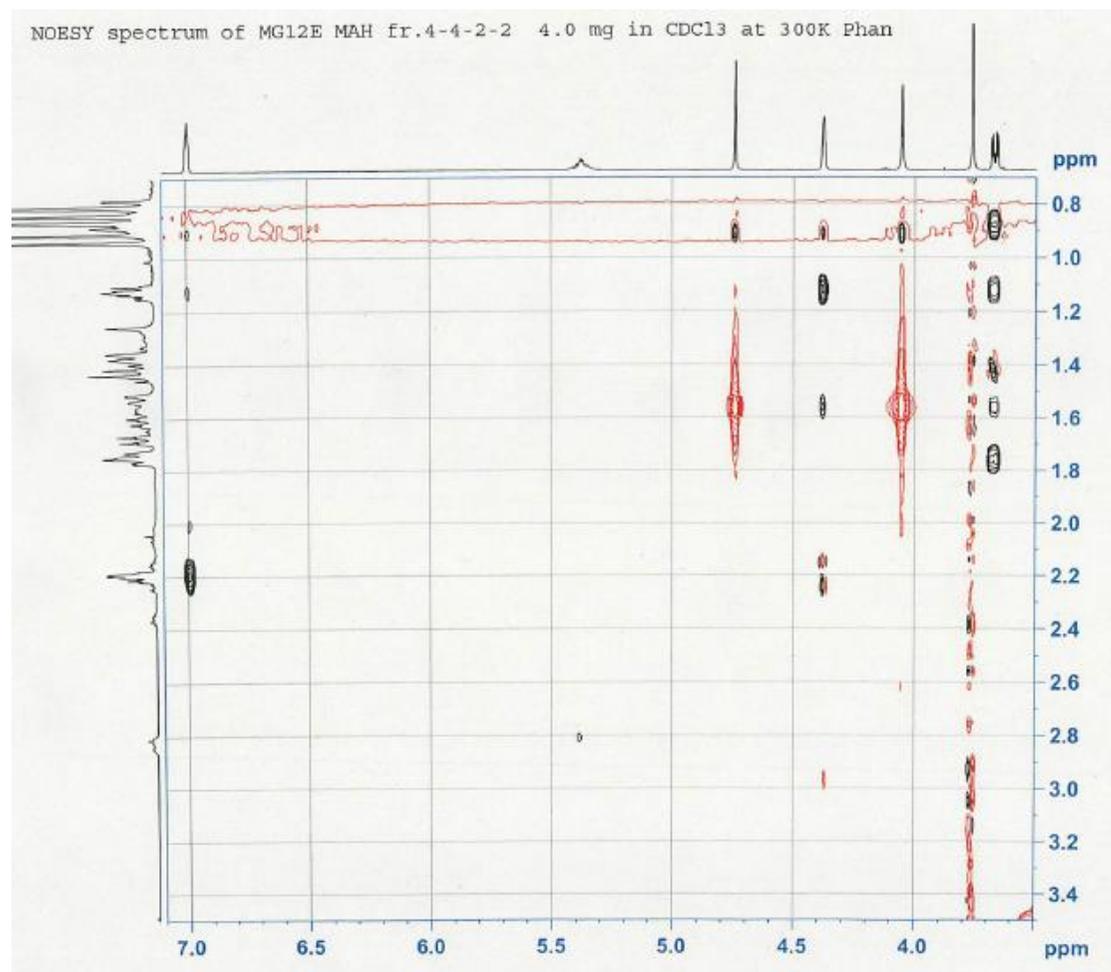
S22: ^1H - ^1H COSY spectrum of **4** in CDCl_3 .



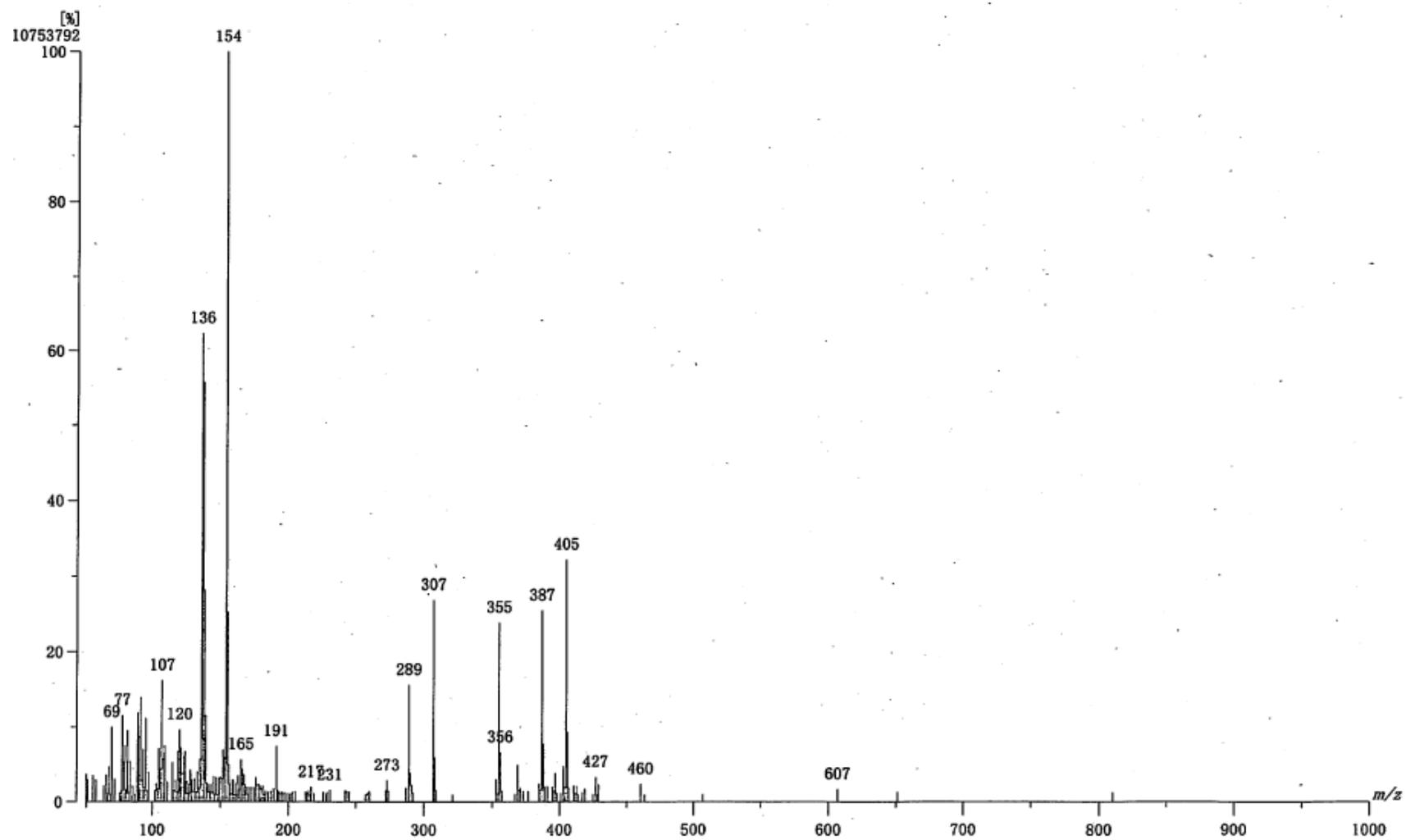
S23: HMBC spectrum of **4** in CDCl₃.



S24: Expanded NOESY spectrum part 1 of 4 in CDCl₃.



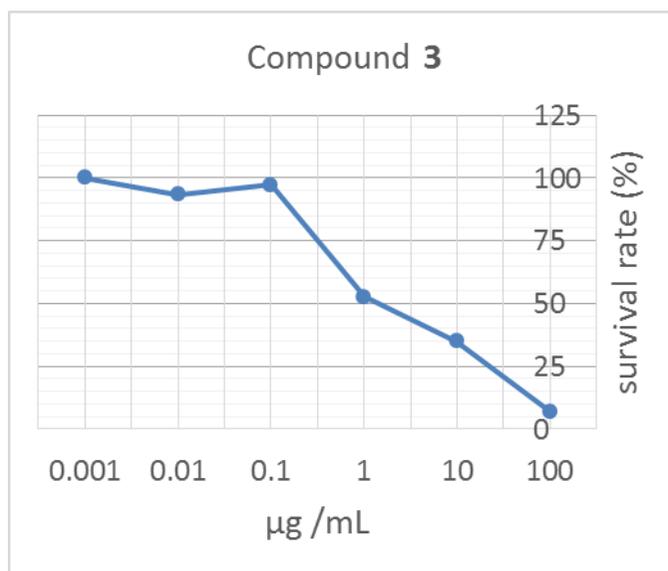
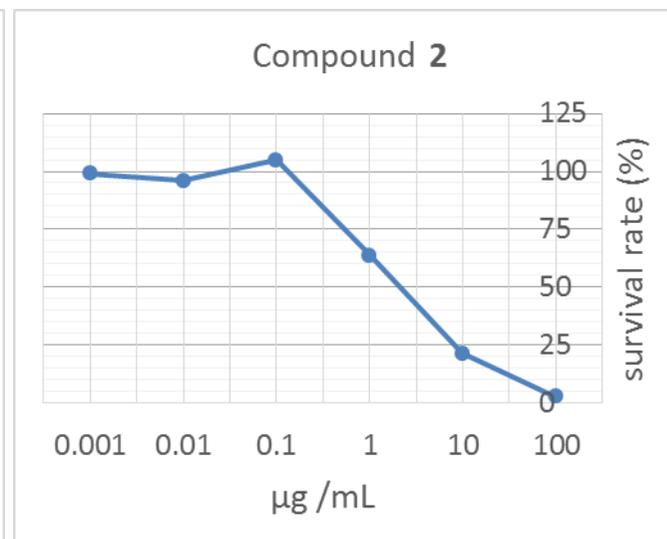
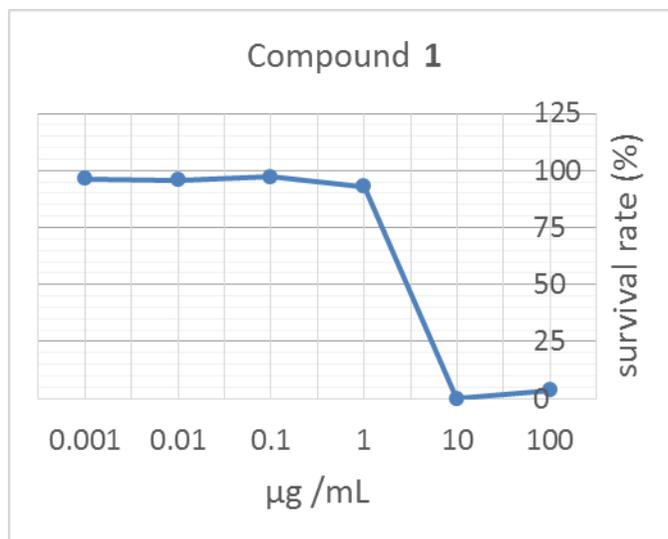
S25: Expanded NOESY spectrum part 2 of 4 in CDCl₃.



S26: FABMS spectrum of 4.

m/z	Int.	Norm.	
201	11.52	1.12	120832
202	11.61	1.13	121728
203	13.82	1.35	144896
205	14.46	1.41	151637
213	14.47	1.41	151765
214	12.65	1.23	132693
215	15.40	1.50	161450
216	10.48	1.02	109866
217	20.82	2.03	218282
219	12.01	1.17	125909
226	13.75	1.34	144170
228	10.86	1.06	113877
229	13.38	1.30	140288
231	16.61	1.62	174122
242	16.06	1.57	168448
243	15.54	1.52	162944
244	13.66	1.33	143189
245	14.18	1.38	148650
257	10.75	1.05	112682
258	11.95	1.16	125269
259	13.17	1.28	138069
260	15.41	1.50	161621
272	16.45	1.60	172458
273	30.03	2.93	314922
274	16.22	1.58	170069
287	19.96	1.95	209322
289	160.29	15.63	1680725
290	40.69	3.97	426624
291	24.34	2.37	255189
292	13.16	1.28	137984
307	275.53	26.87	2889173
308	61.20	5.97	641706
309	16.98	1.66	178090
321	10.26	1.00	107562
353	31.70	3.09	332416
354	12.25	1.19	128426
355	244.83	23.87	2567253
356	68.50	6.68	718250
357	16.17	1.58	169600
367	11.23	1.10	117802
369	51.18	4.99	536704
370	17.14	1.67	179712
371	19.51	1.90	204629
373	14.84	1.45	155648
377	14.78	1.44	155008
385	25.19	2.46	264106

386	17.75	1.73	186112
387	261.29	25.48	2739840
388	79.62	7.76	834901
389	20.41	1.99	214016
391	21.91	2.14	229717
395	21.08	2.06	221056
396	15.69	1.53	164522
397	39.85	3.89	417834
398	12.74	1.24	133546
401	12.23	1.19	128256
403	48.72	4.75	510848
404	20.77	2.03	217813
405	330.48	32.22	3465301
406	95.78	9.34	1004373
407	19.84	1.93	208085
411	22.51	2.19	236032
412	12.13	1.18	127146
413	21.82	2.13	228821
414	10.81	1.05	113322
417	13.18	1.29	138240
419	18.35	1.79	192426
425	10.68	1.04	112000
427	34.33	3.35	359936
428	10.45	1.02	109525
429	24.31	2.37	254933
460	24.97	2.43	261802
463	10.42	1.02	109269
507	10.73	1.05	112469
607	17.98	1.75	188501
651	13.80	1.35	144725
810	13.67	1.33	143317



S27: Cytotoxicity of **1-3** against adult T-cell leukemia, S1T cells.