Supplementary materials

Anti-inflammatory and cytotoxic potential of new phenanthrenoids from *Luzula sylvatica*

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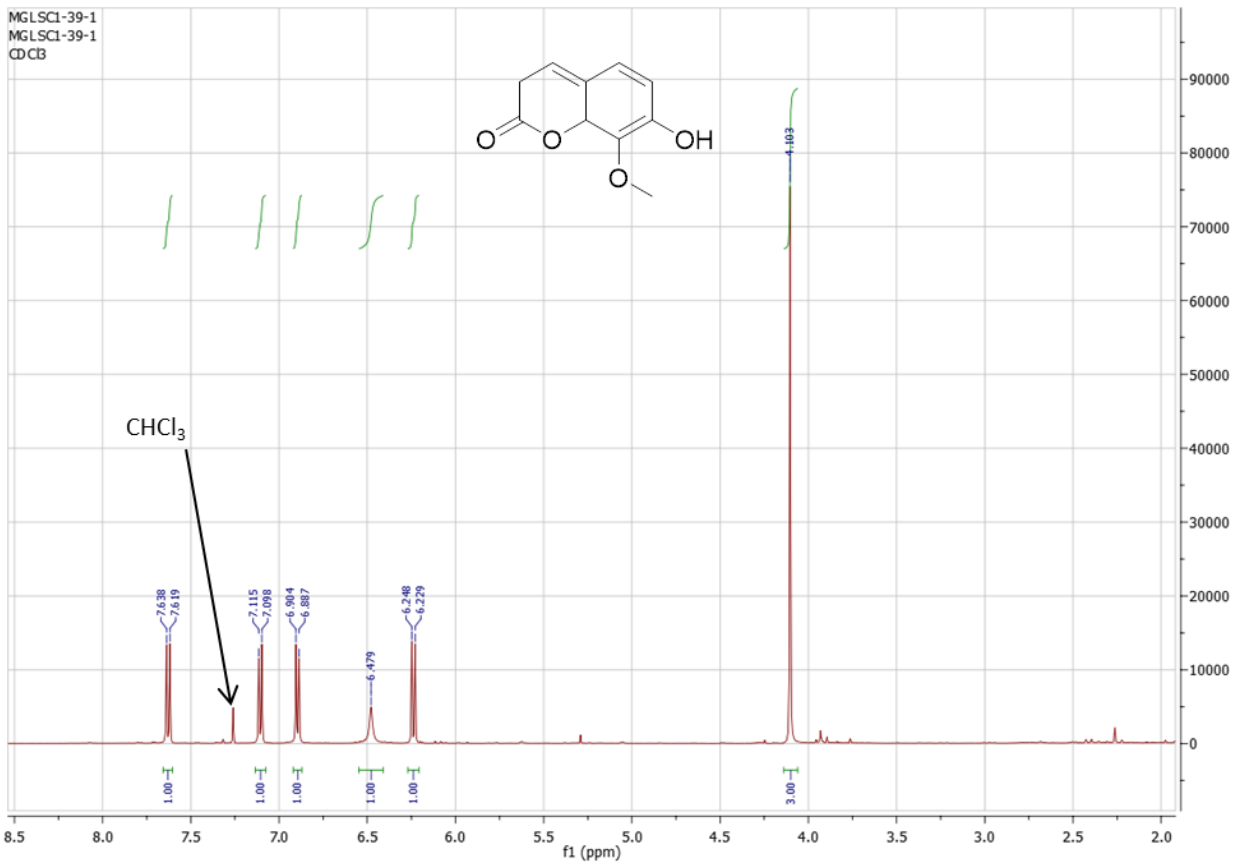

Figure S1. ^{1}H-NMR spectrum of hydrangetin (**1**) (500MHz, $CDCl_3$)

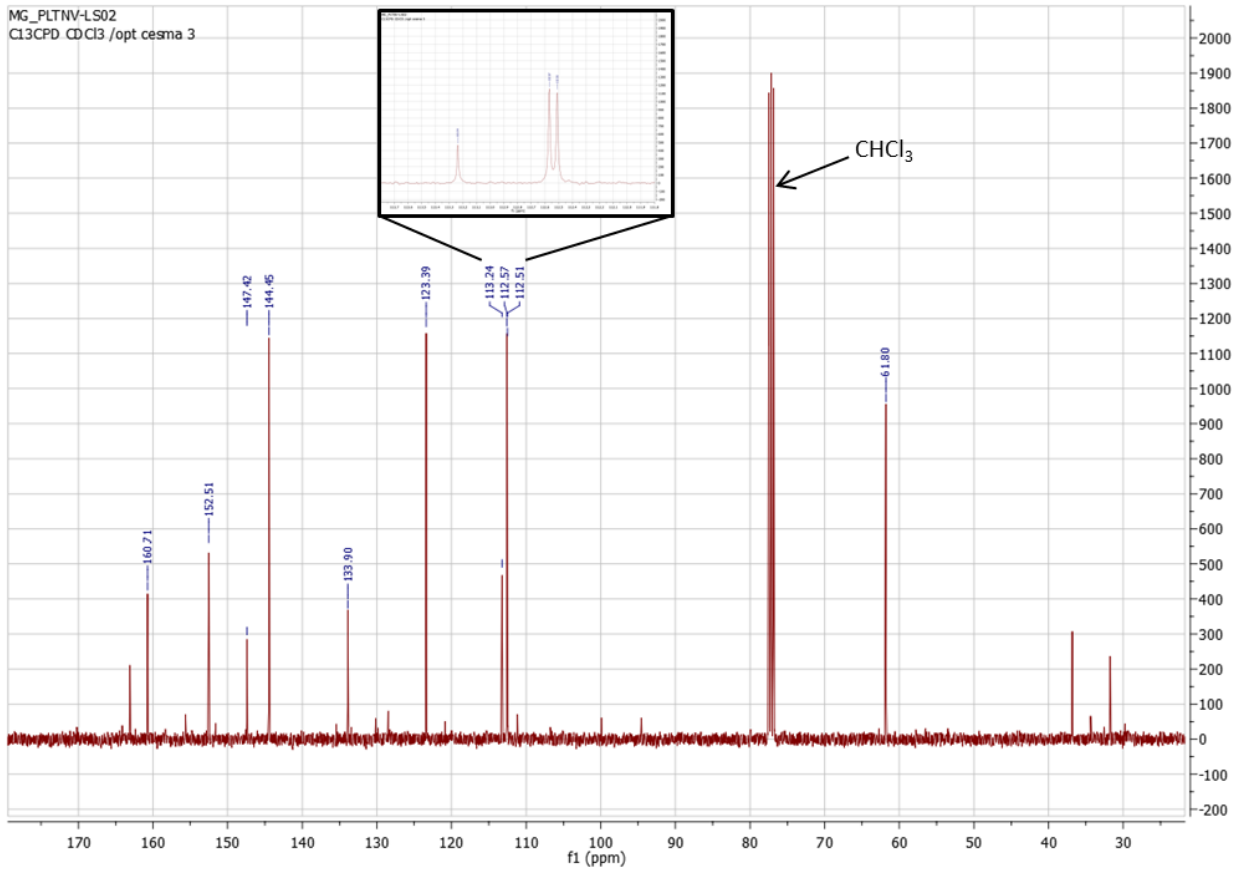

Figure S2. ^{13}C-NMR Spectrum of hydrangetin (**1**) (100MHz, $CDCl_3$)

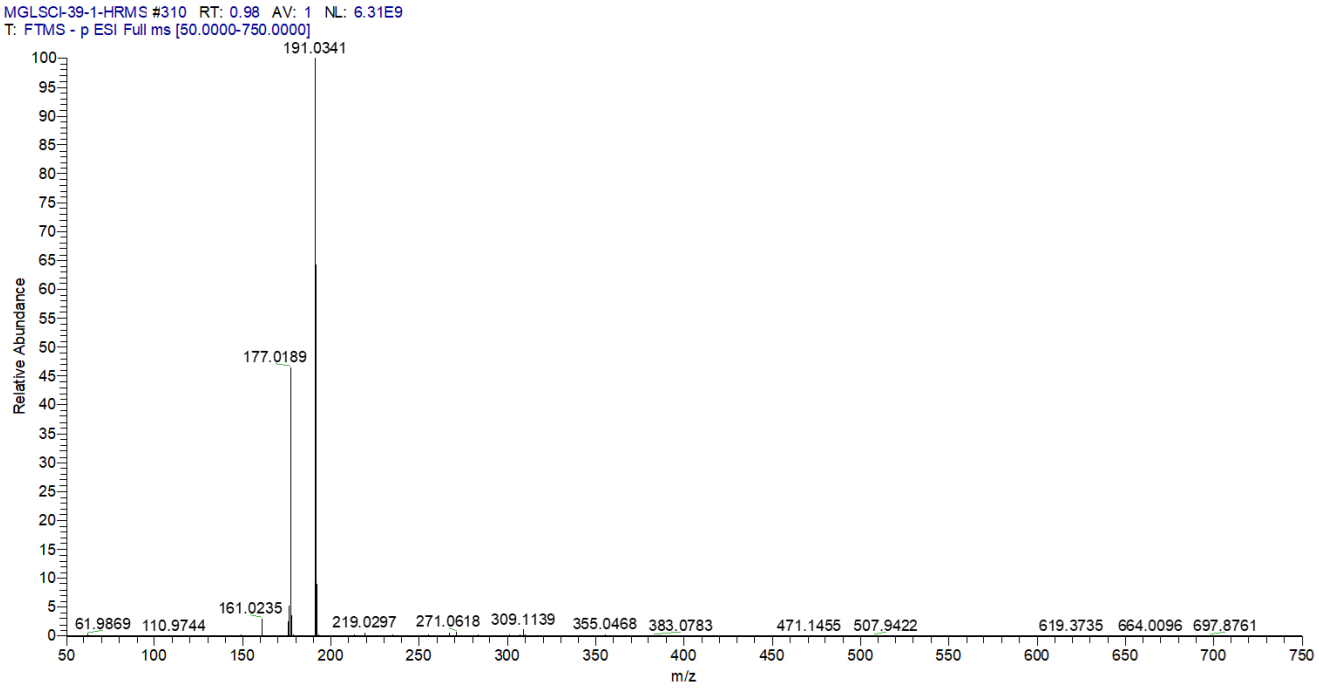

Figure S3. HRESIMS of hydrangetin (1) (negative ionisation mode)

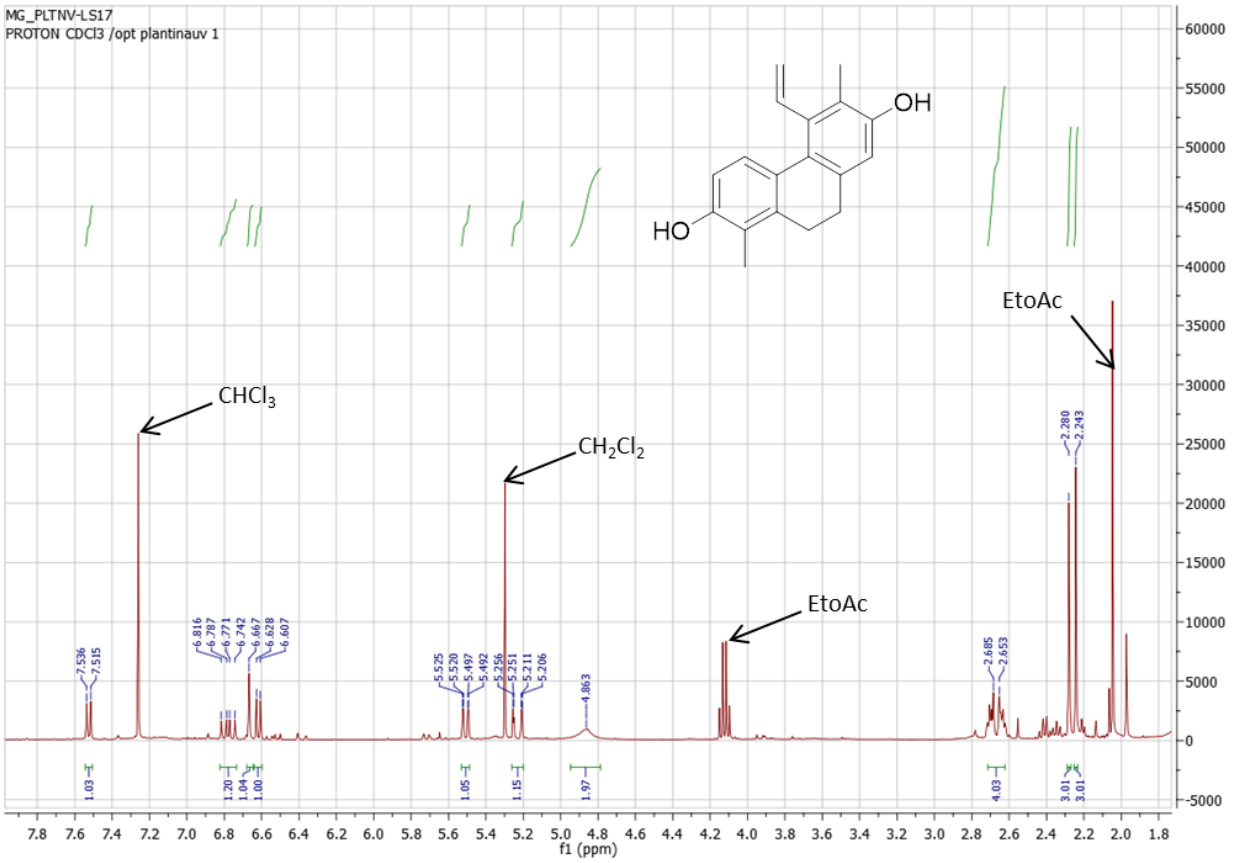

Figure S4. ^{1}H-NMR spectrum of juncusol (2) (400MHz, $CDCl_3$)

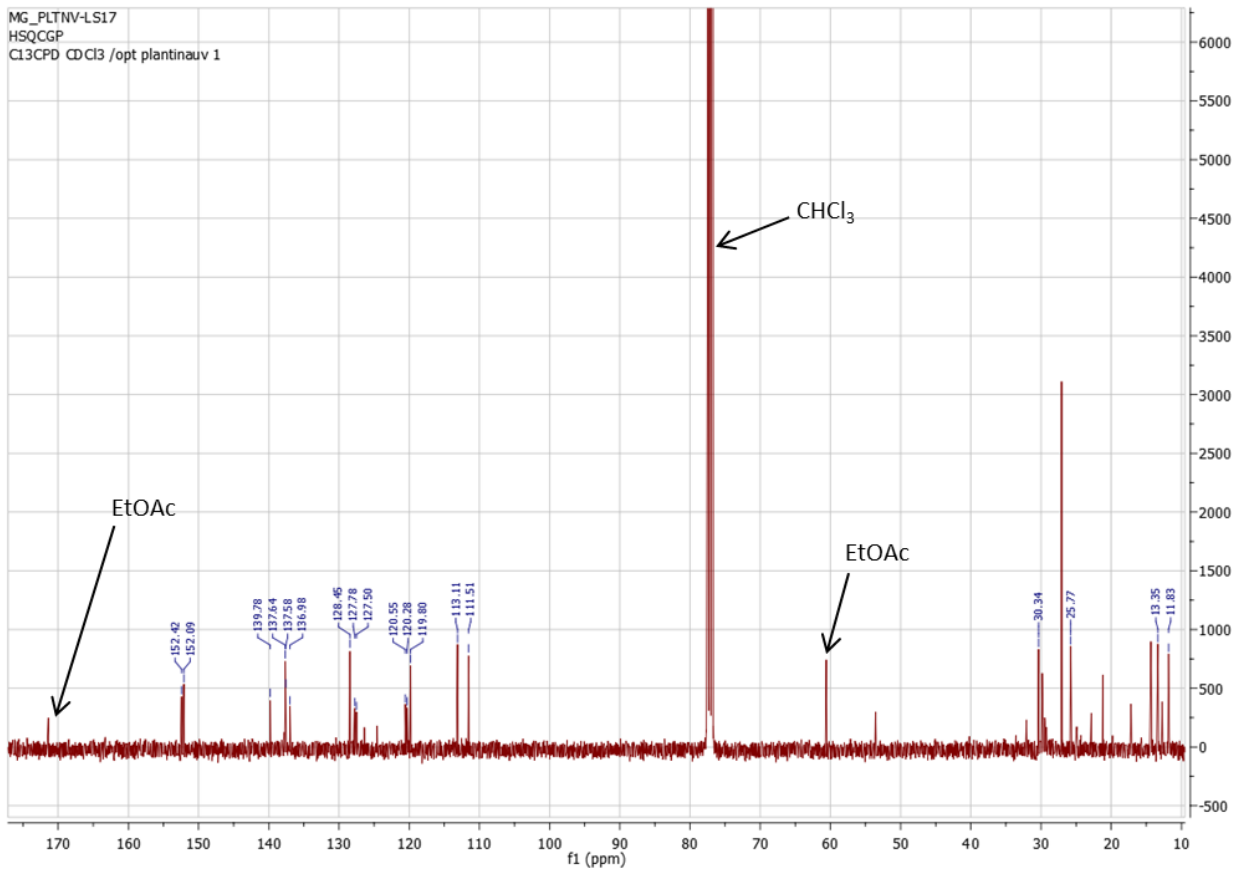

Figure S5. ^{13}C-NMR spectrum of juncusol (**2**) (100MHz, $CDCl_3$)

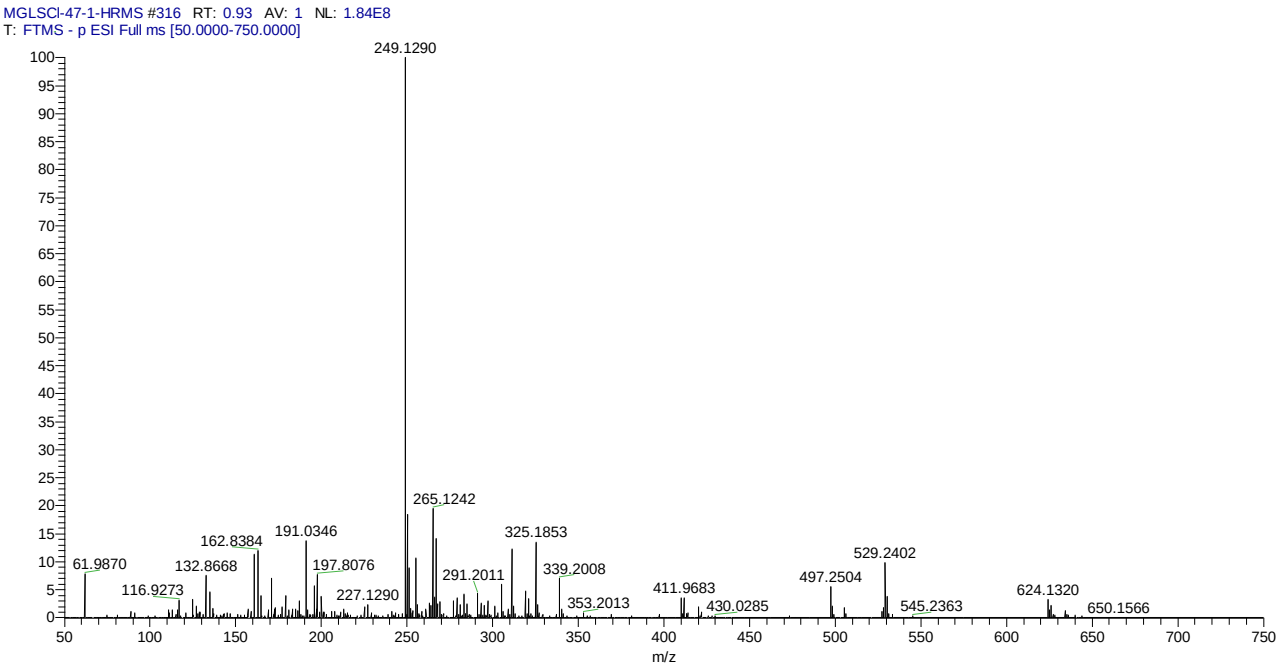

Figure S6. HRESIMS of juncusol (**2**) (negative ionisation mode)

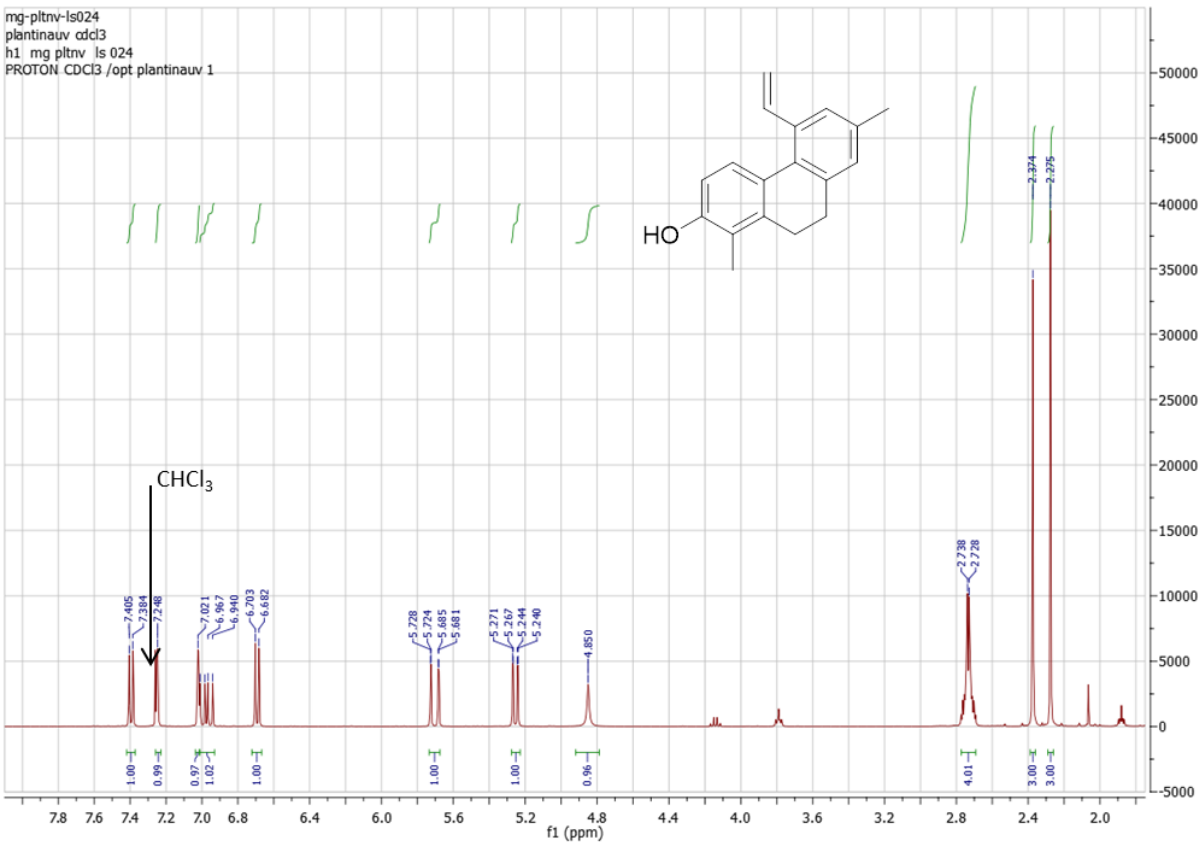

Figure S7. ^{1}H-NMR spectrum of juncunol (**3**) (400MHz, $CDCl_3$)

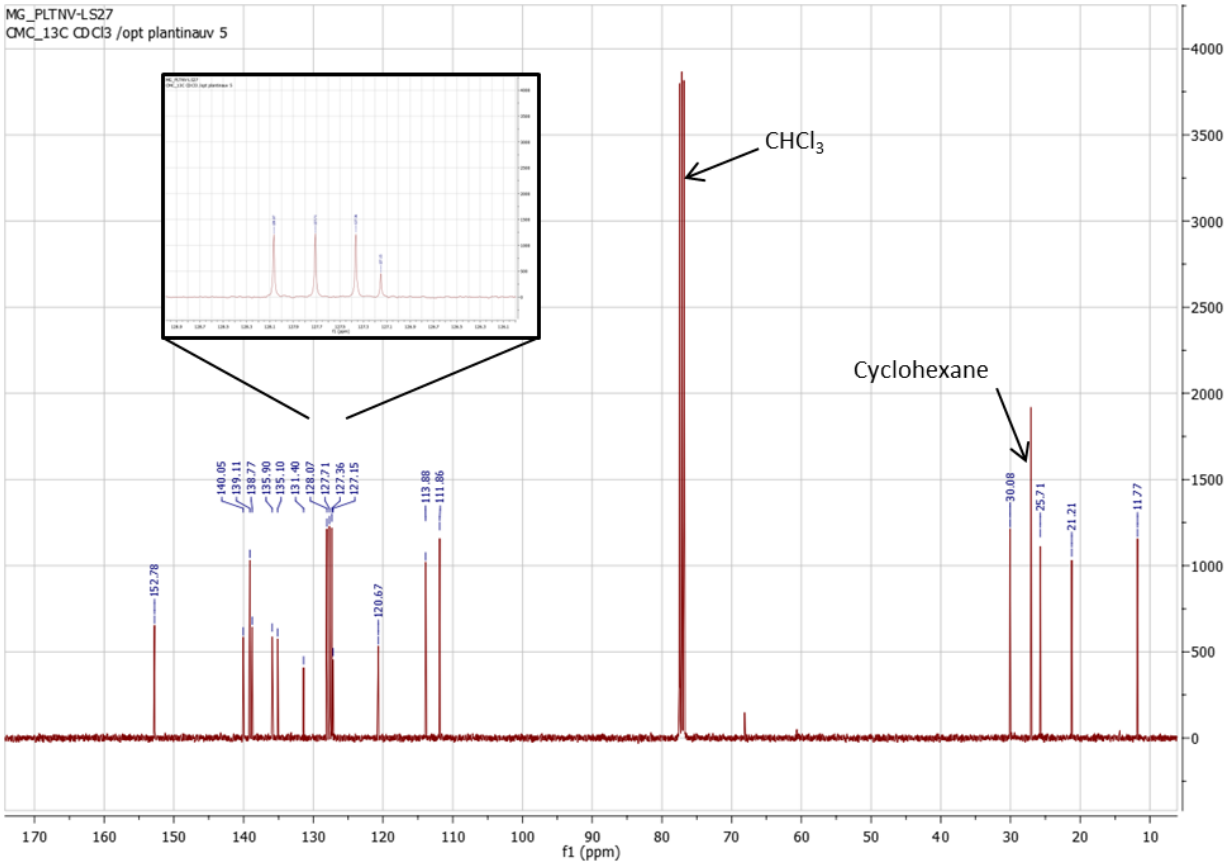

Figure S8. ^{13}C-NMR spectrum of juncunol (**3**) (100MHz, $CDCl_3$)

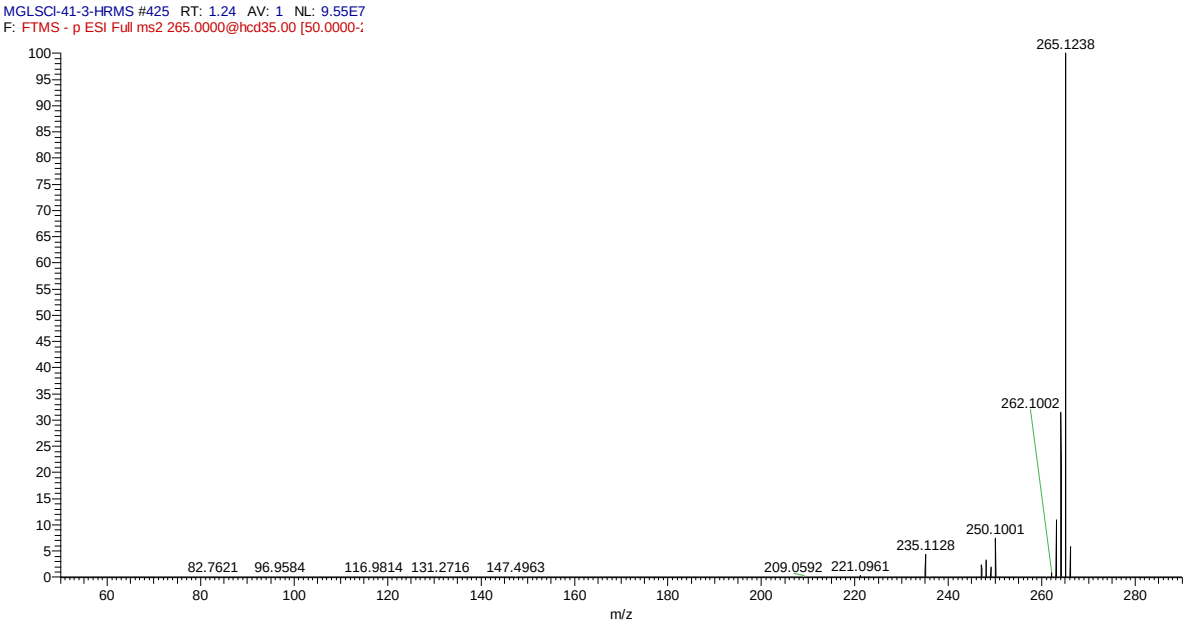

Figure S9. HRESIMS of juncunol (**3**) (negative ionisation mode)

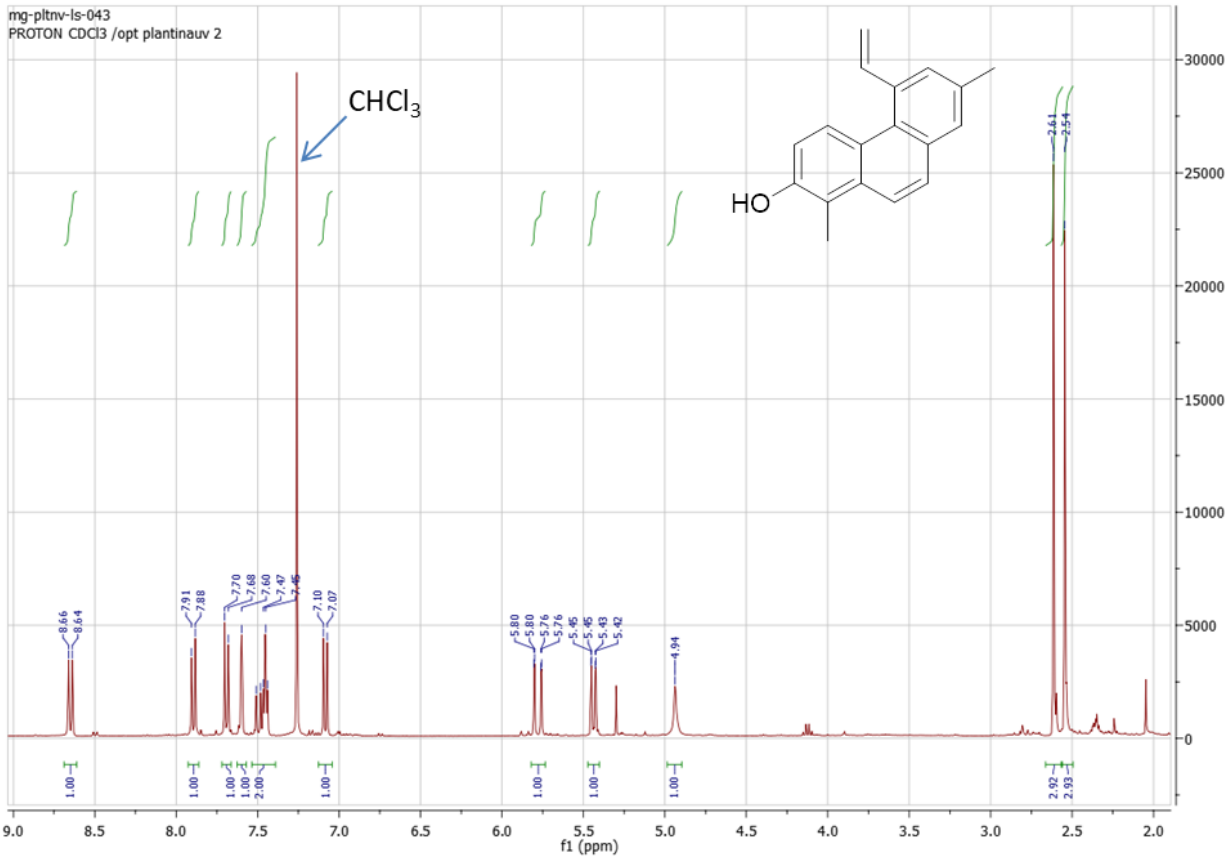

Figure S10. ^{1}H-NMR spectrum of 1,7-dimethyl-5-vinyl phenanthren-2-ol (**4**) (400MHz, $CDCl_3$)

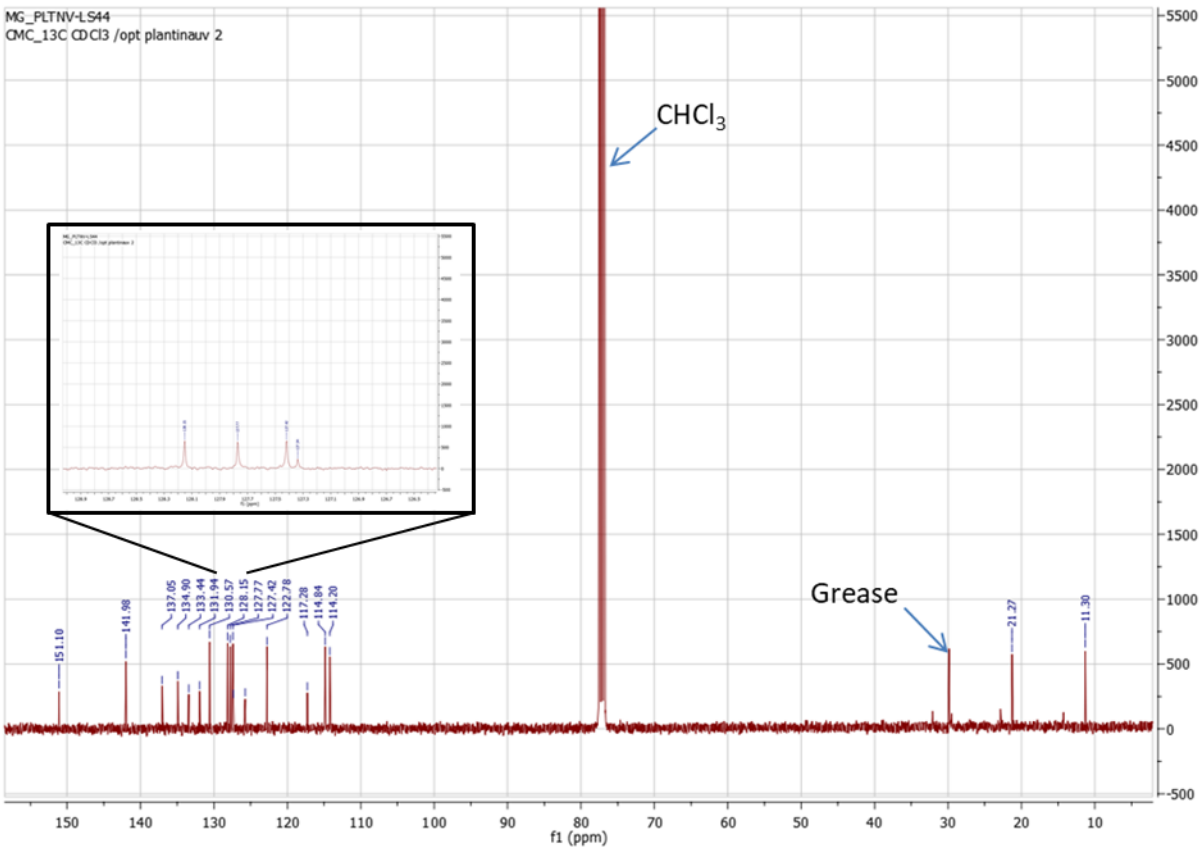

Figure S11. ^{13}C-NMR spectrum of 1,7-dimethyl-5-vinyl phenanthren-2-ol (**4**) (100MHz, $CDCl_3$)

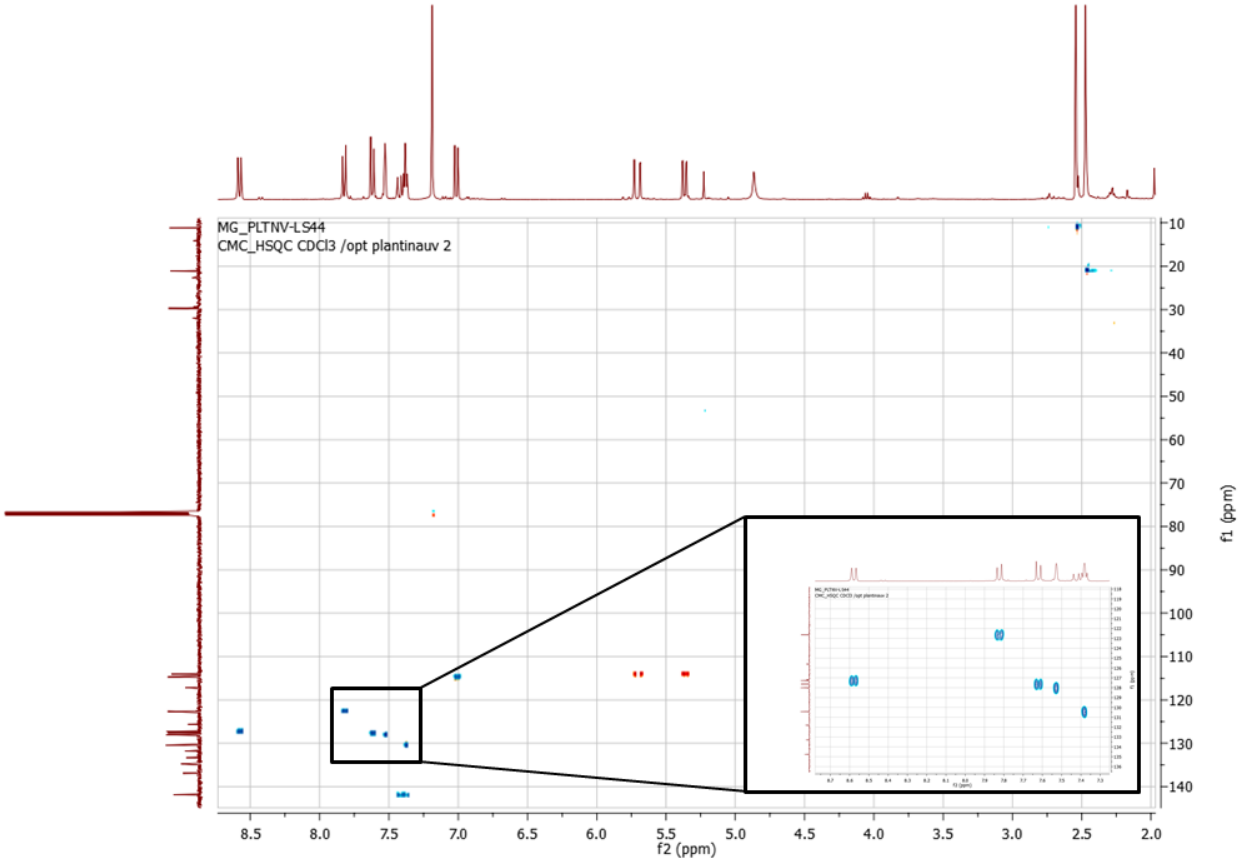

Figure S12. ^{1}H-^{13}C HSQC spectrum of 1,7-dimethyl-5-vinyl phenanthren-2-ol (**4**) (400MHz, $CDCl_3$)

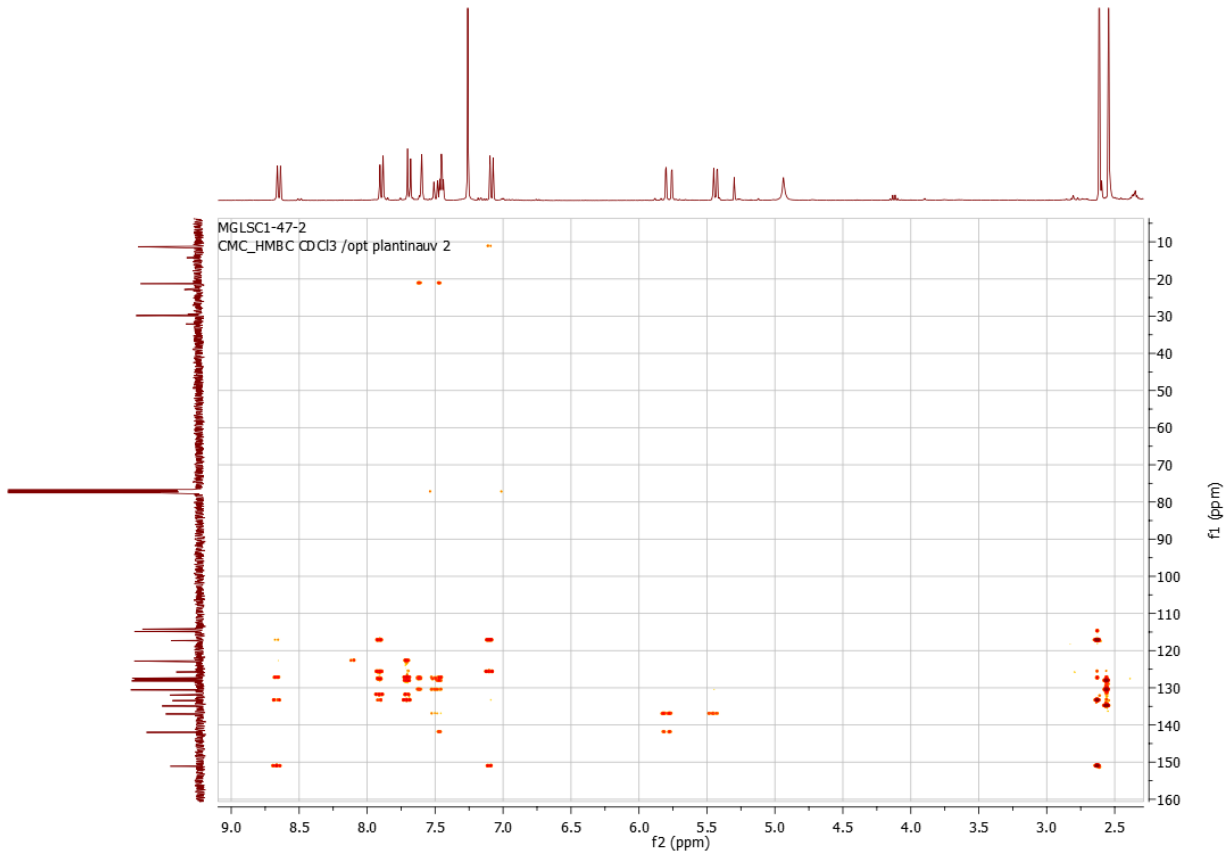

Figure S13. ^{1}H-^{13}C HMBC spectrum of 1,7-dimethyl-5-vinyl phenanthren-2-ol (**4**) (400MHz, $CDCl_3$)

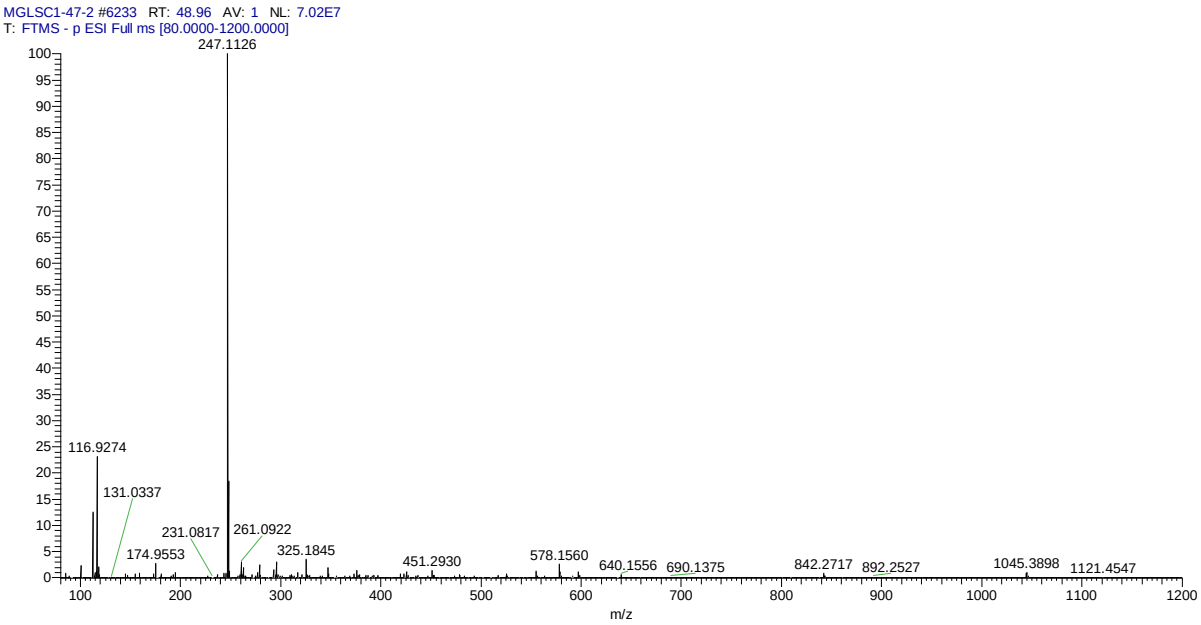

Figure S14. HRESIMS of 1,7-dimethyl-5-vinyl phenanthren-2-ol (**4**) (negative ionisation mode)

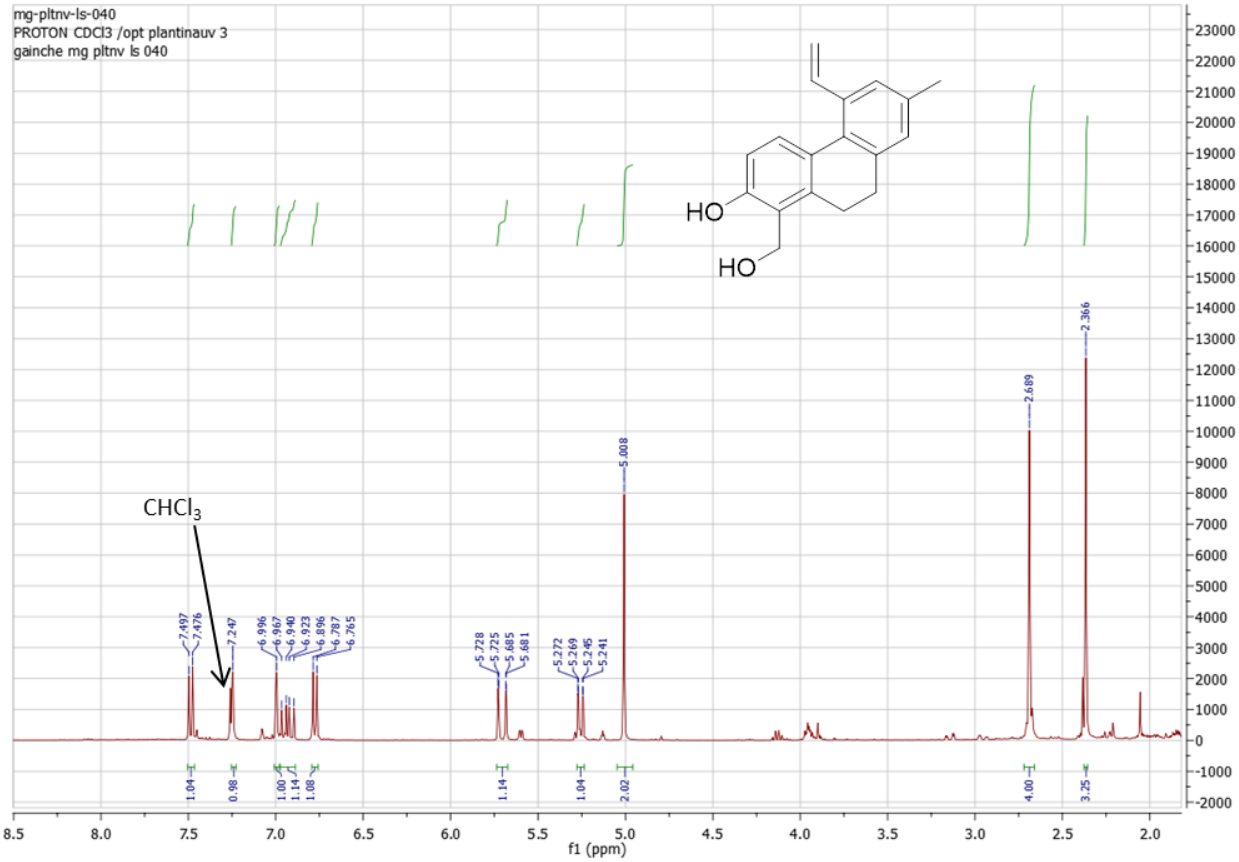

Figure S15. ^{1}H-NMR spectrum of 1-hydroxymethyl-7-methyl-5-vinyl-9,10-hydrophenanthren-2-ol (**5**) (400MHz, $CDCl_3$)

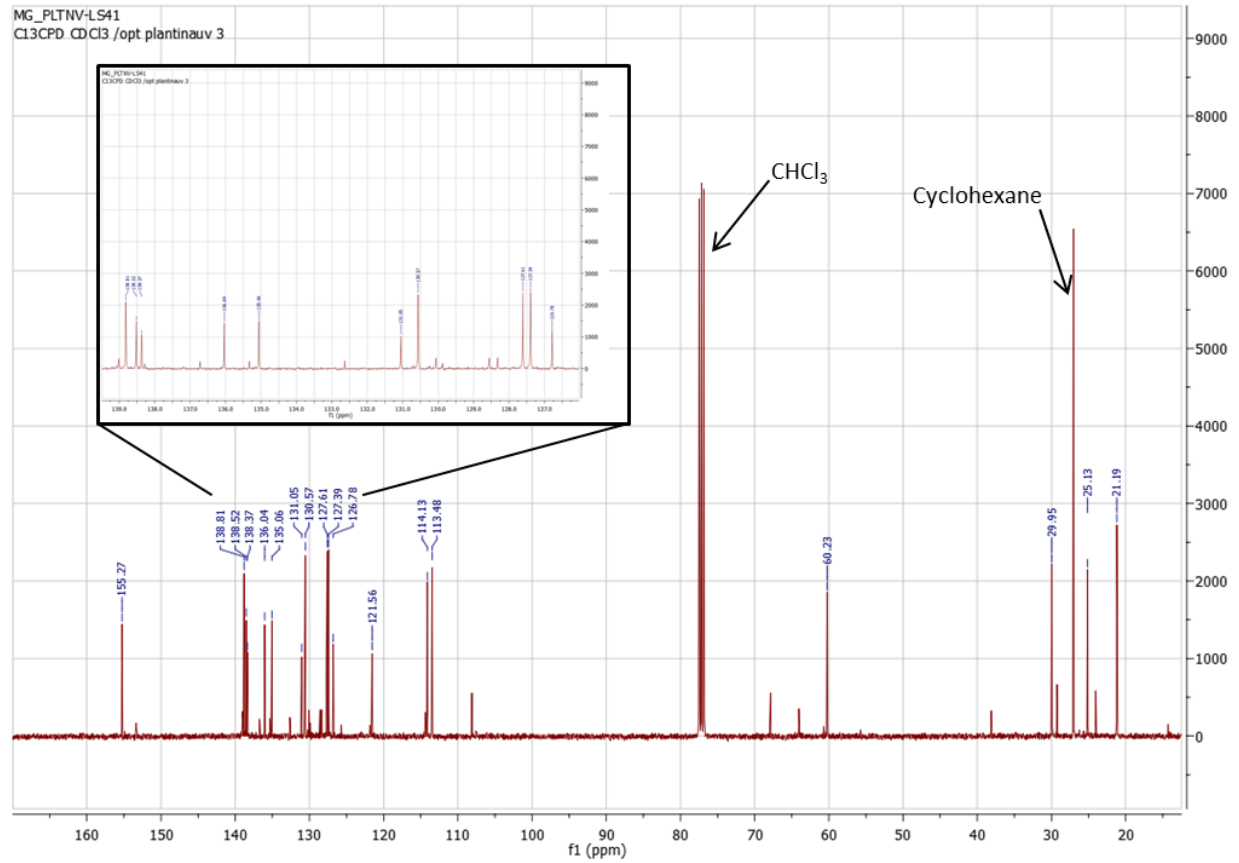

Figure S16. ^{13}C-NMR spectrum of 1-hydroxymethyl-7-methyl-5-vinyl-9,10-hydrophenanthren-2-ol (**5**) (100MHz, $CDCl_3$)

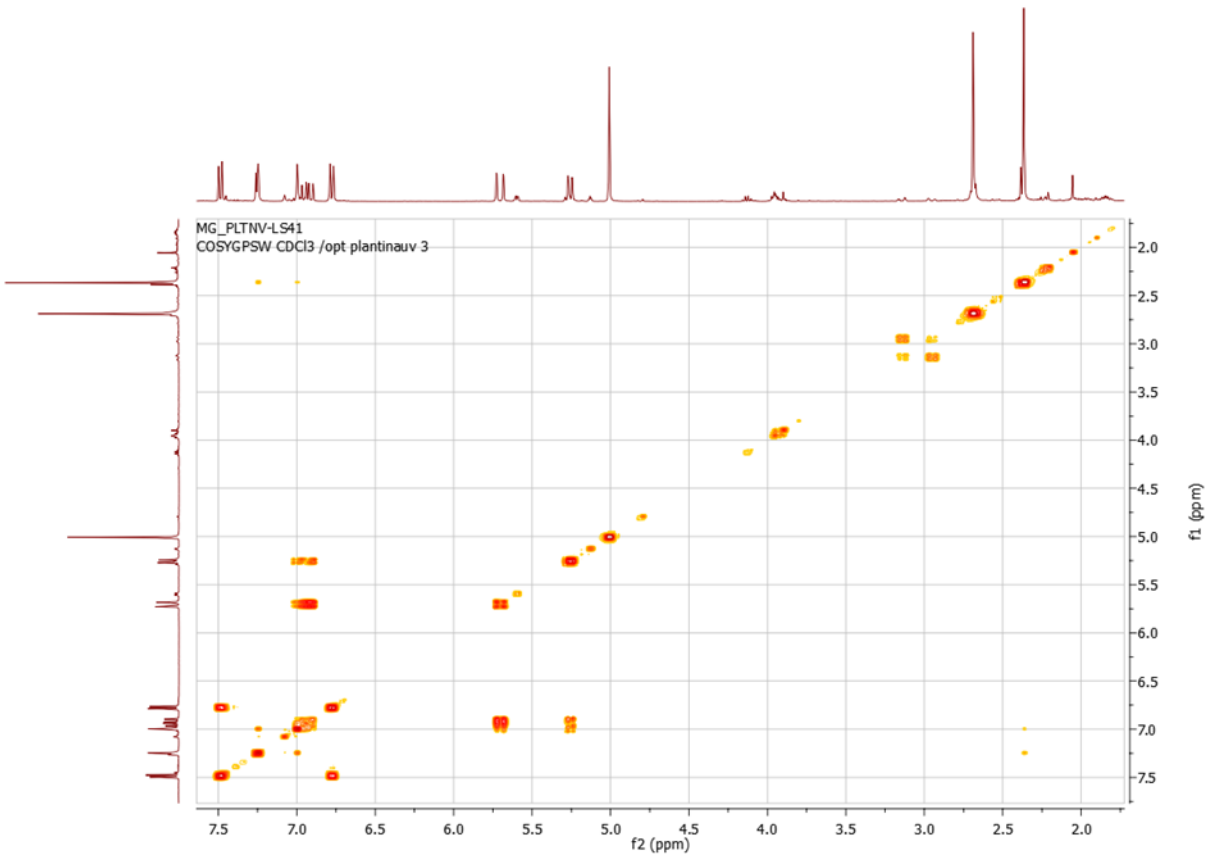

Figure S17. ^{1}H-^{1}H COSY spectrum of 1-hydroxymethyl-7-methyl-5-vinyl-9,10-hydrophenanthren-2-ol (**5**) (400MHz, $CDCl_3$)

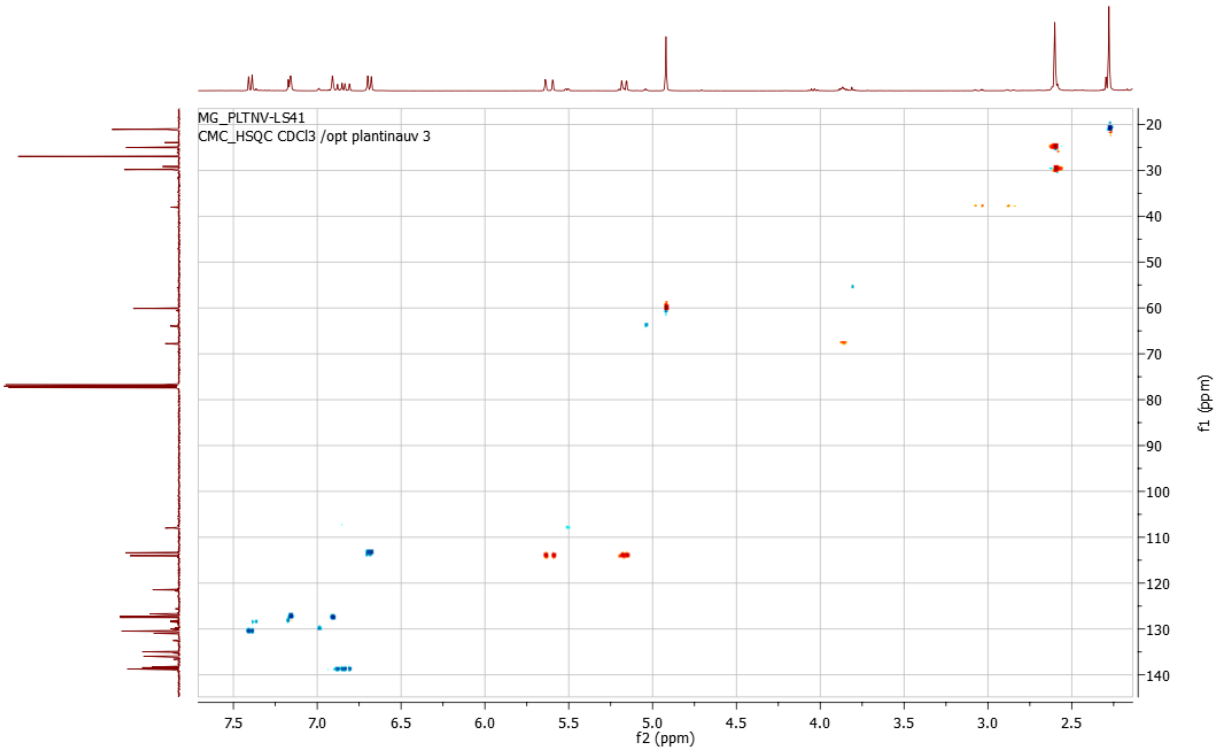

Figure S18. ^{1}H-^{13}C HSQC spectrum of 1-hydroxymethyl-7-methyl-5-vinyl-9,10-hydrophenanthren-2-ol (**5**) (400MHz, $CDCl_3$)

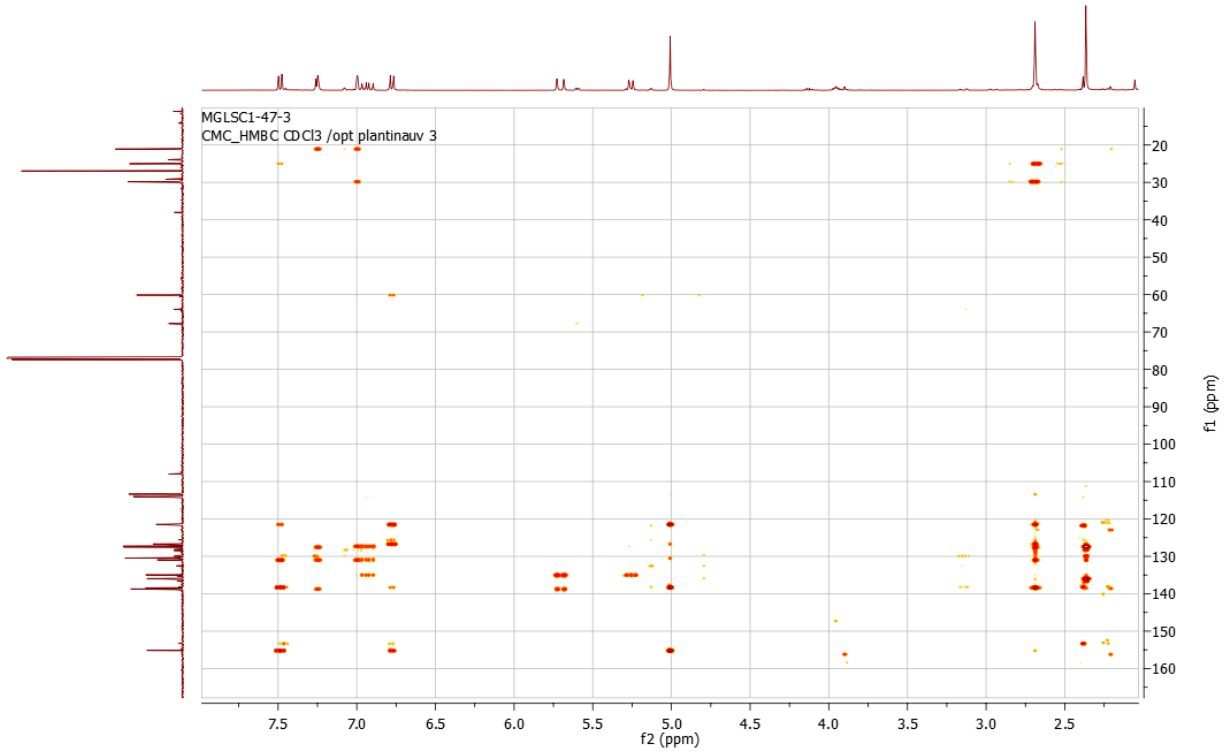

Figure S19. ^{1}H-^{13}C HMBC spectrum of 1-hydroxymethyl-7-methyl-5-vinyl-9,10-hydrophenanthren-2-ol (**5**) (400MHz, $CDCl_3$)

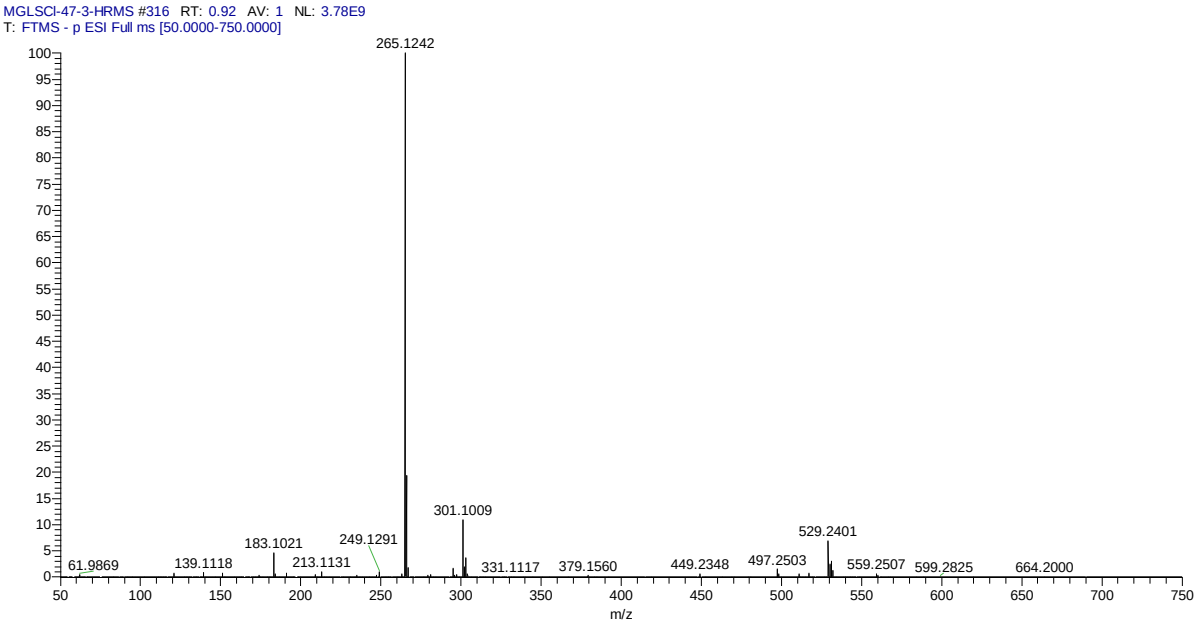

Figure S20. HRESIMS of 1-hydroxymethyl-7-methyl-5-vinyl-9,10-hydrophenanthren-2-ol (**5**) (negative ionisation mode)

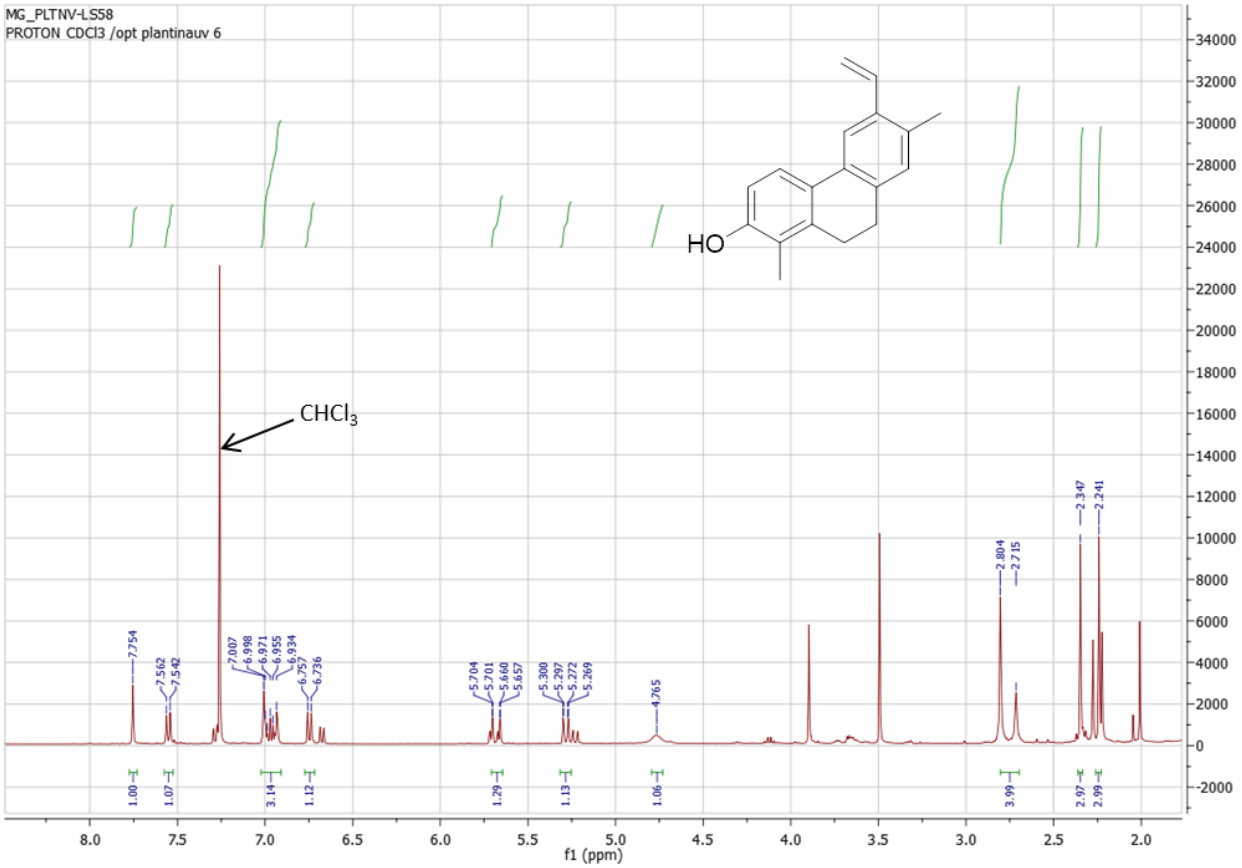

Figure S21. ^{1}H-NMR spectrum of juncuenin A (**6**) (400MHz, $CDCl_3$)

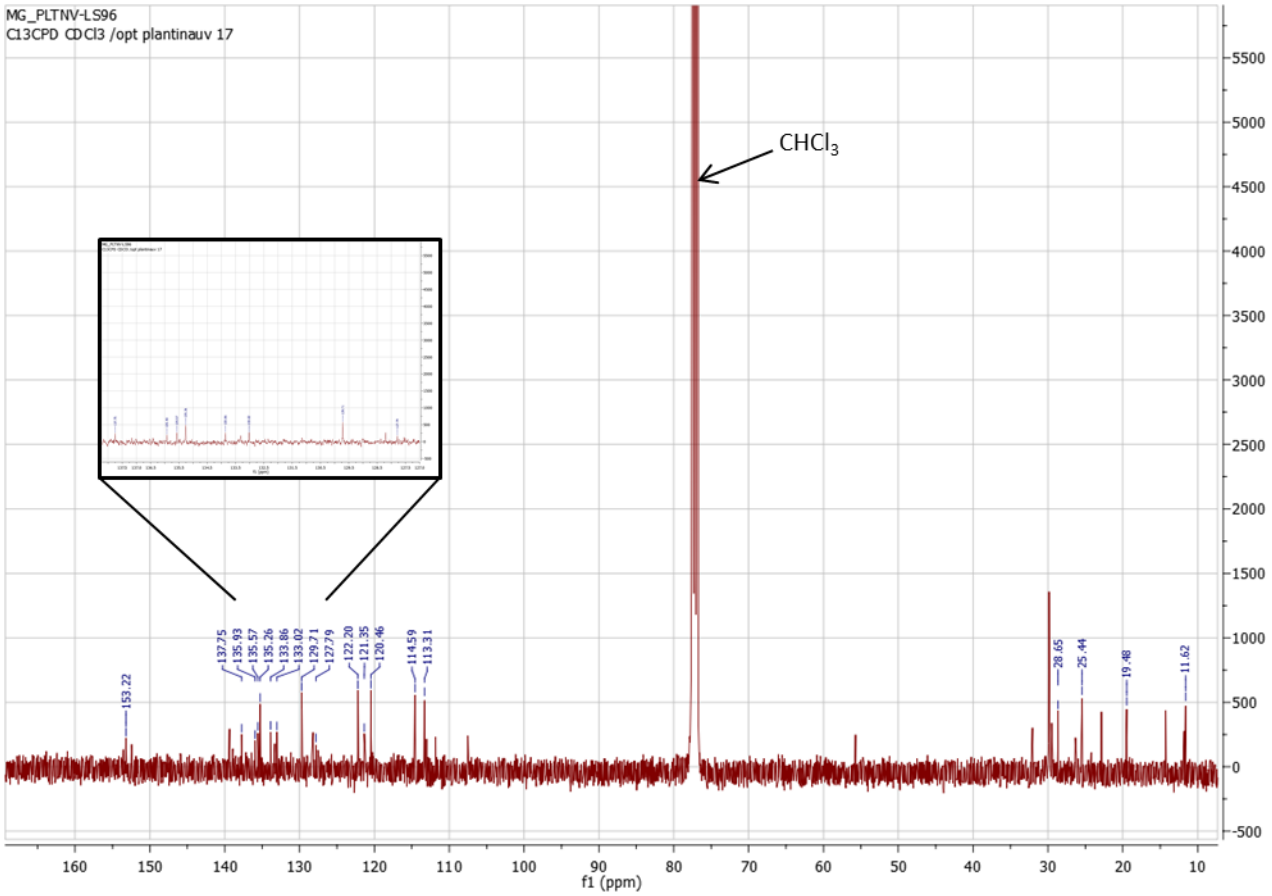

Figure S22. ^{13}C-NMR spectrum of juncuenin A (**6**) (100MHz, $CDCl_3$)

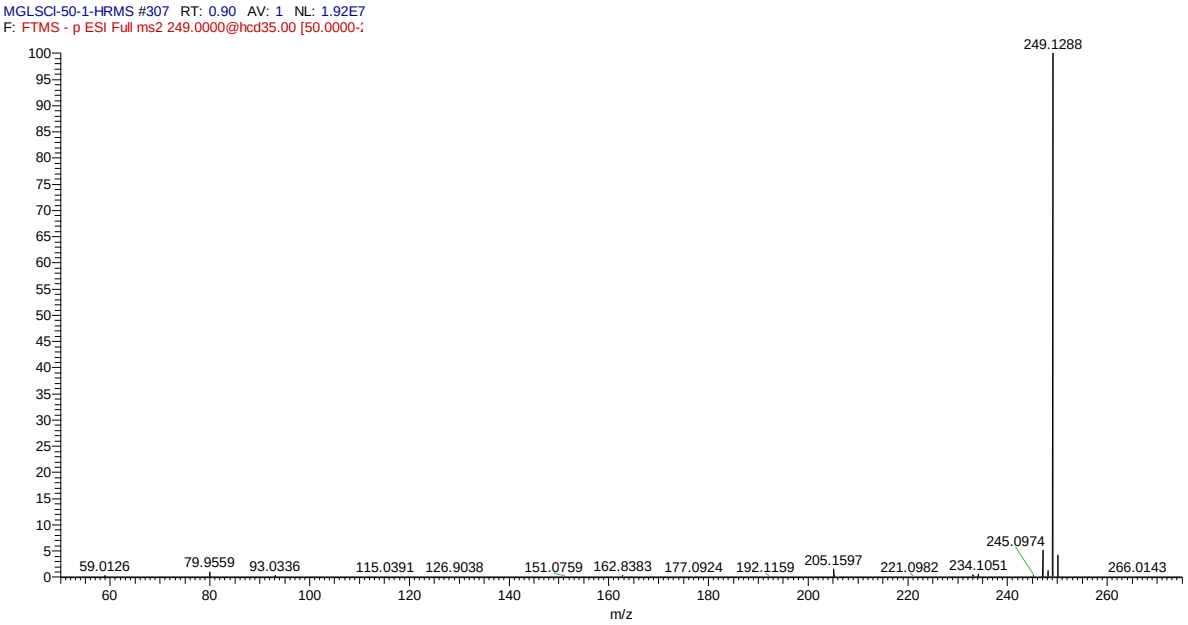

Figure S23. HRESIMS of juncuenin A (**6**) (negative ionisation mode)

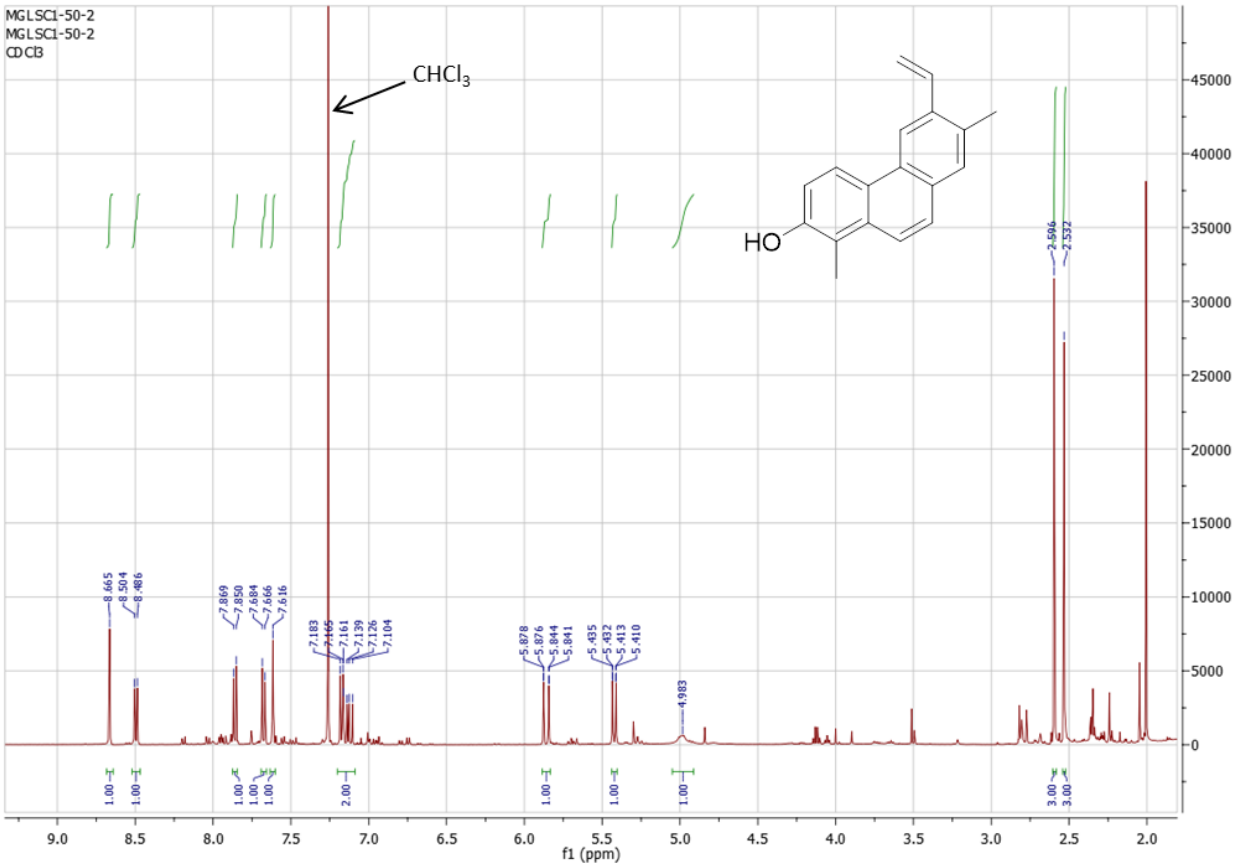

Figure S24. ^{1}H-NMR spectrum of dehydrojucuenin A (**7**) (400MHz, $CDCl_3$)

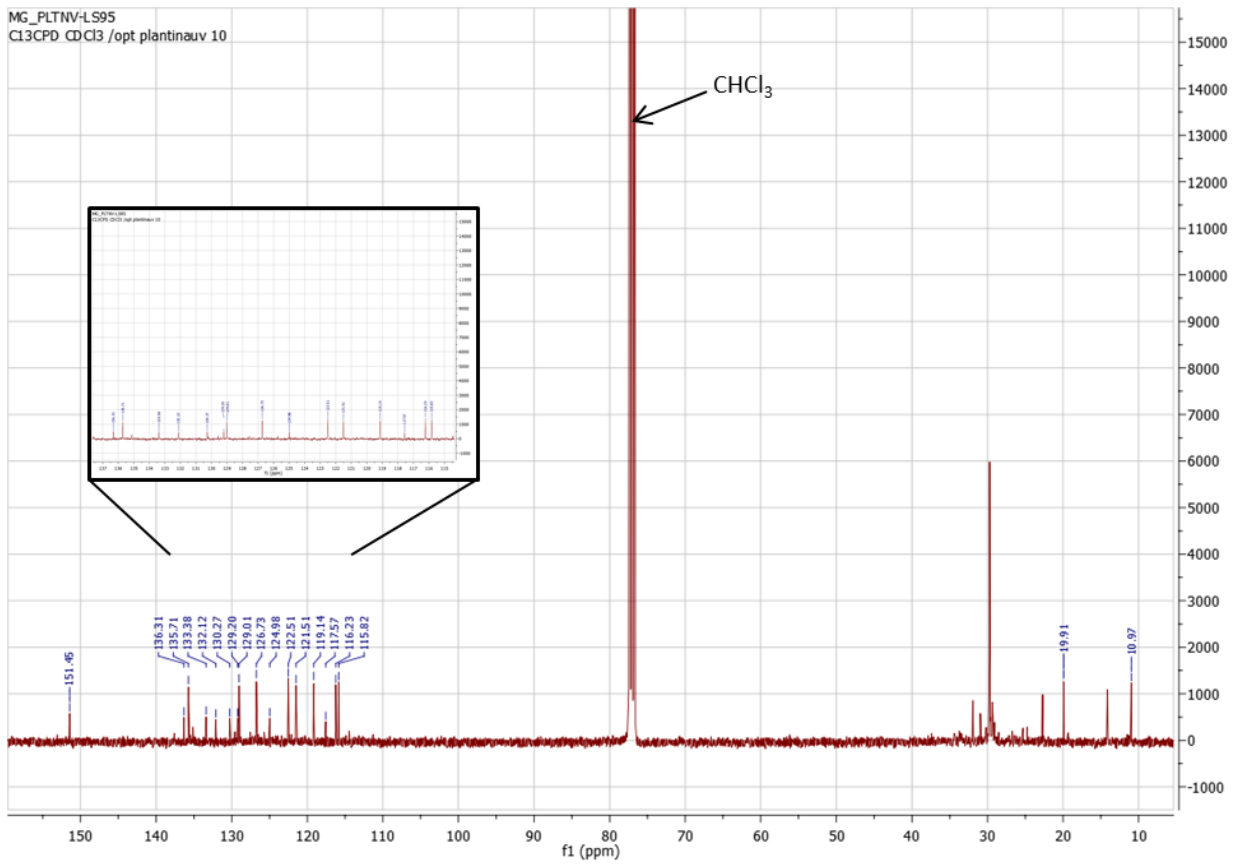

Figure S25. ^{13}C-NMR spectrum of dehydojuncuenin A (**7**) (100MHz, $CDCl_3$)

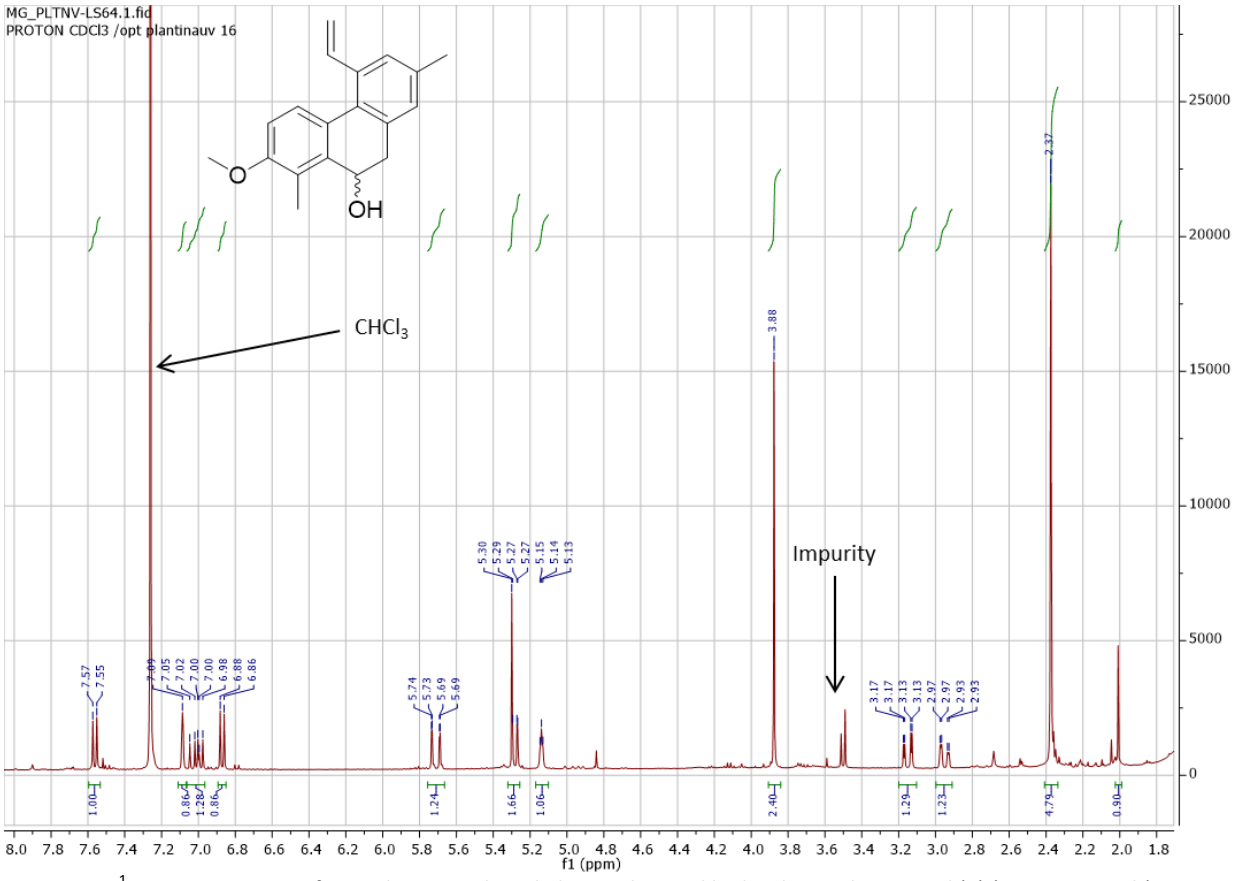

Figure S26. ^{1}H-NMR spectrum of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (**8**) (400MHz, $CDCl_3$)

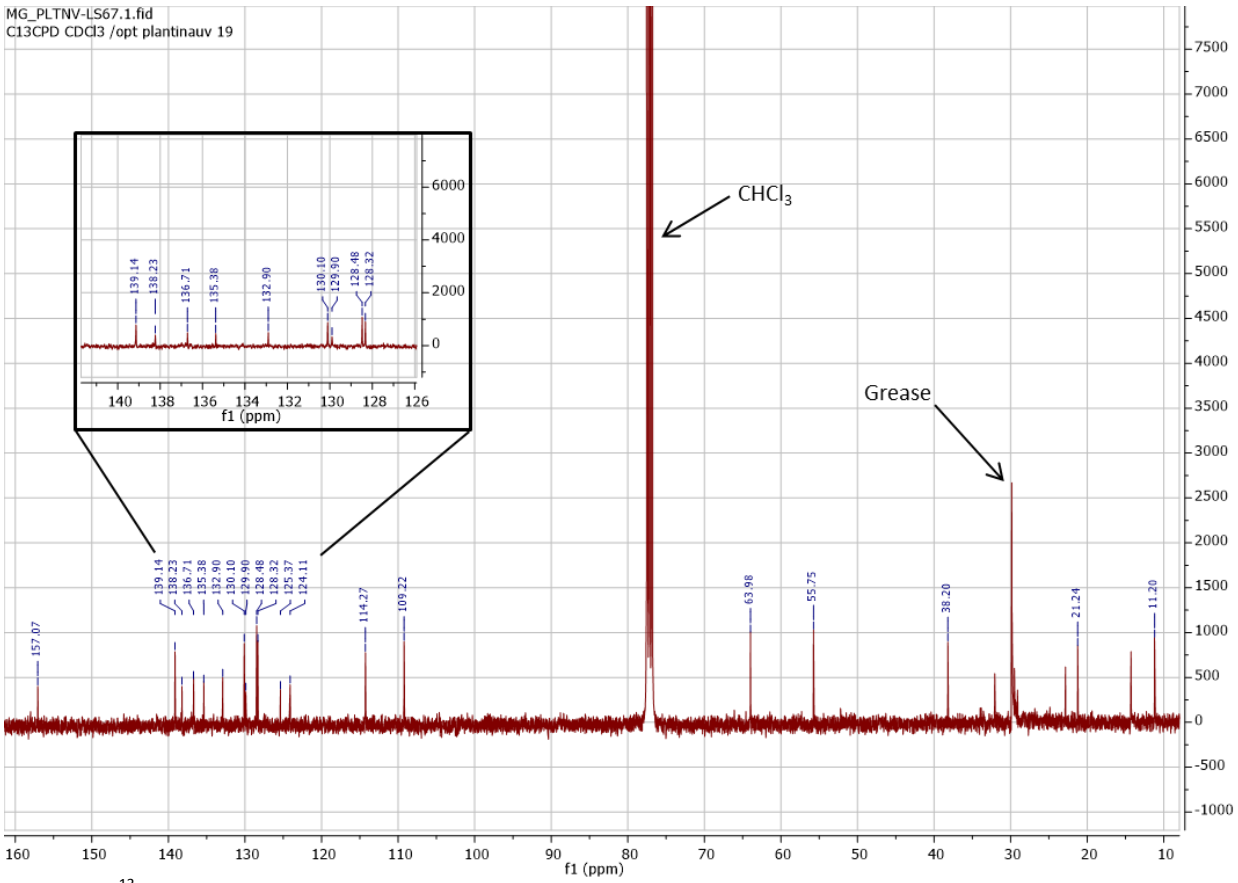

Figure S27. ^{13}C-NMR JMOD spectrum of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (**8**) (100MHz, $CDCl_3$, CH and CH_3 down, C and CH_2 up)

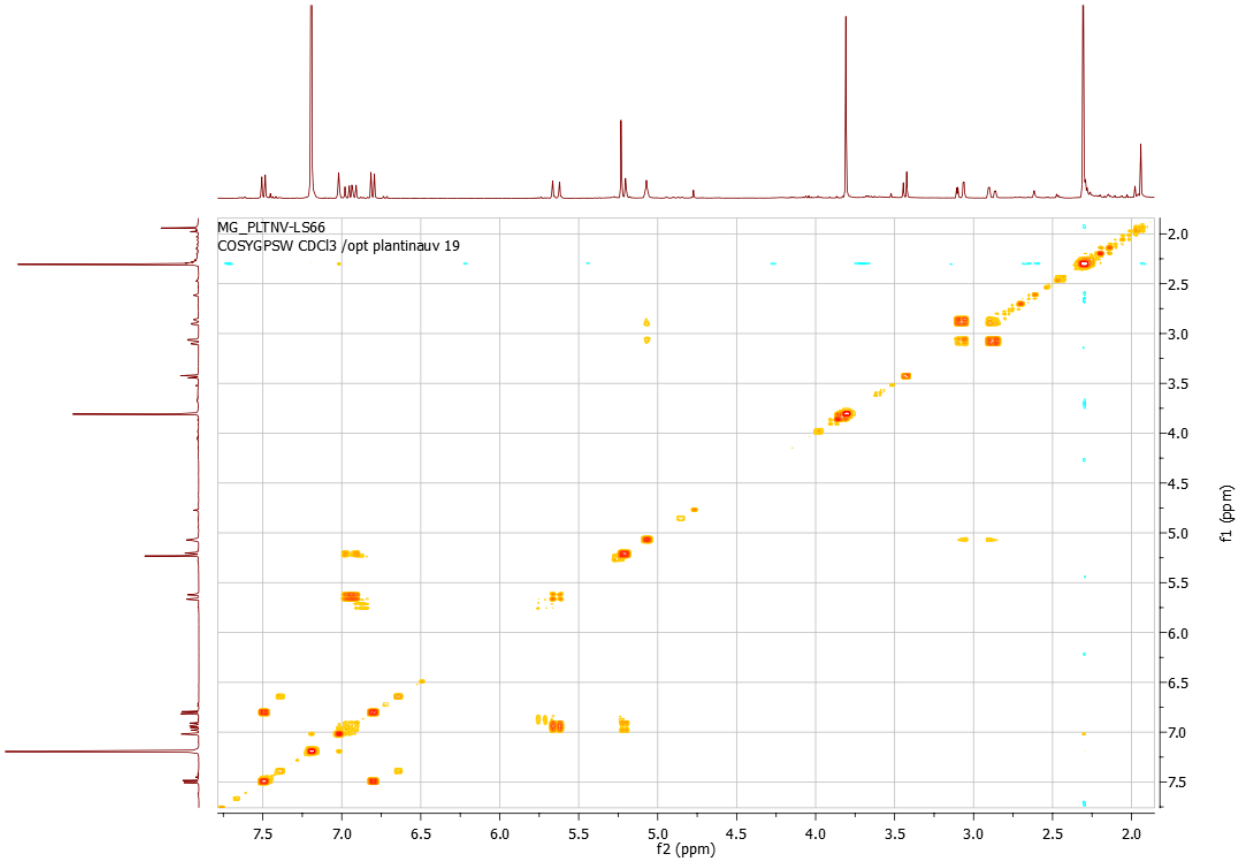

Figure S28. ^{1}H-^{1}H COSY spectrum of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (**8**) (400MHz, $CDCl_3$)

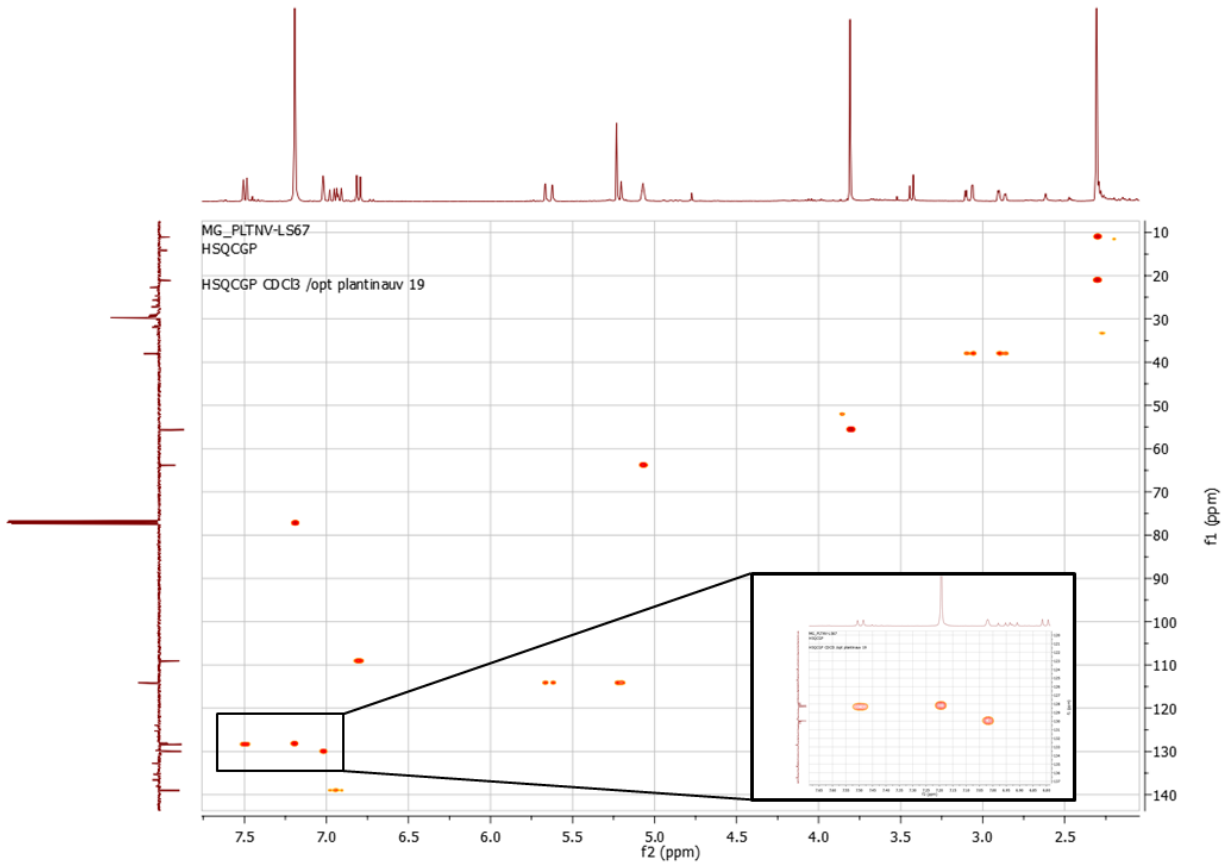

Figure S29. ^{1}H-^{13}C HSQC spectrum of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (**8**) (400MHz, $CDCl_3$)

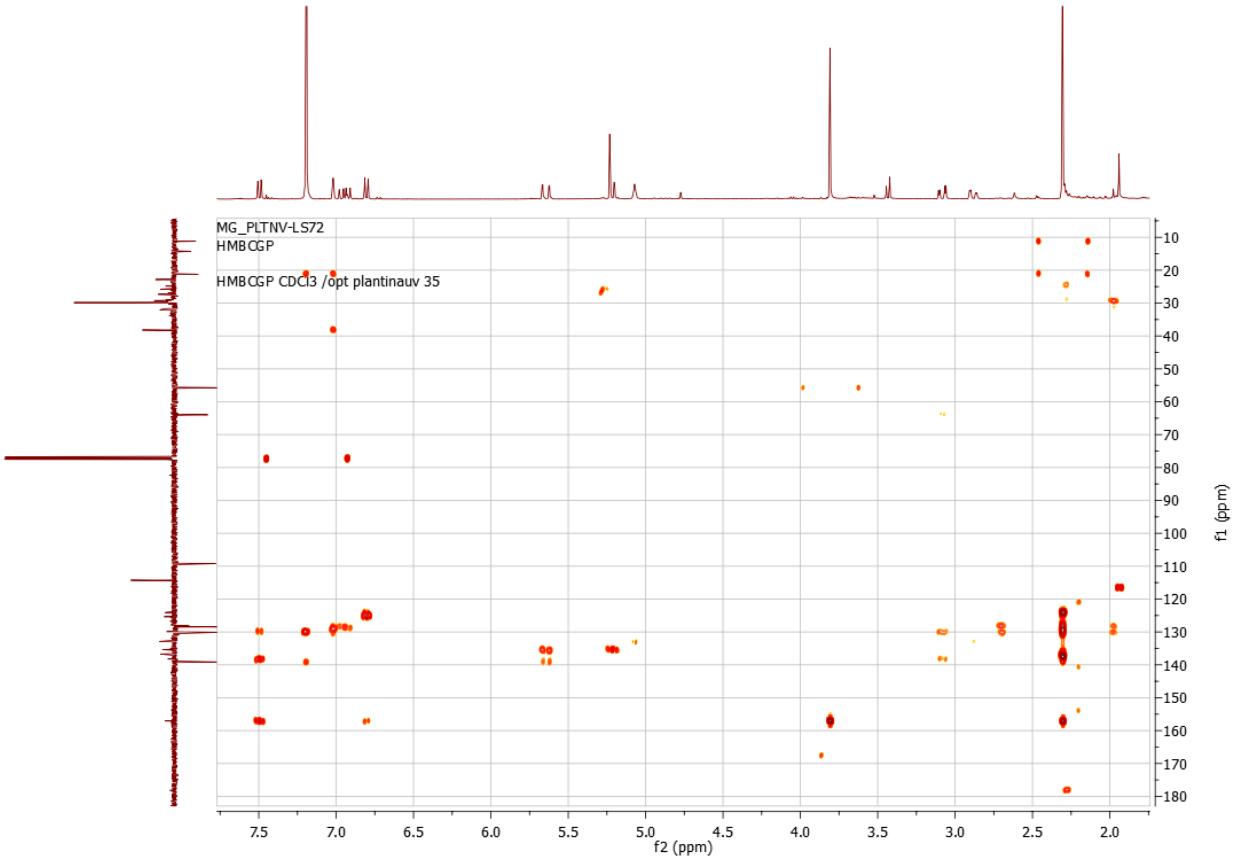

Figure S30. ^{1}H-^{13}C HMBC spectrum of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (**8**) (400MHz, $CDCl_3$)

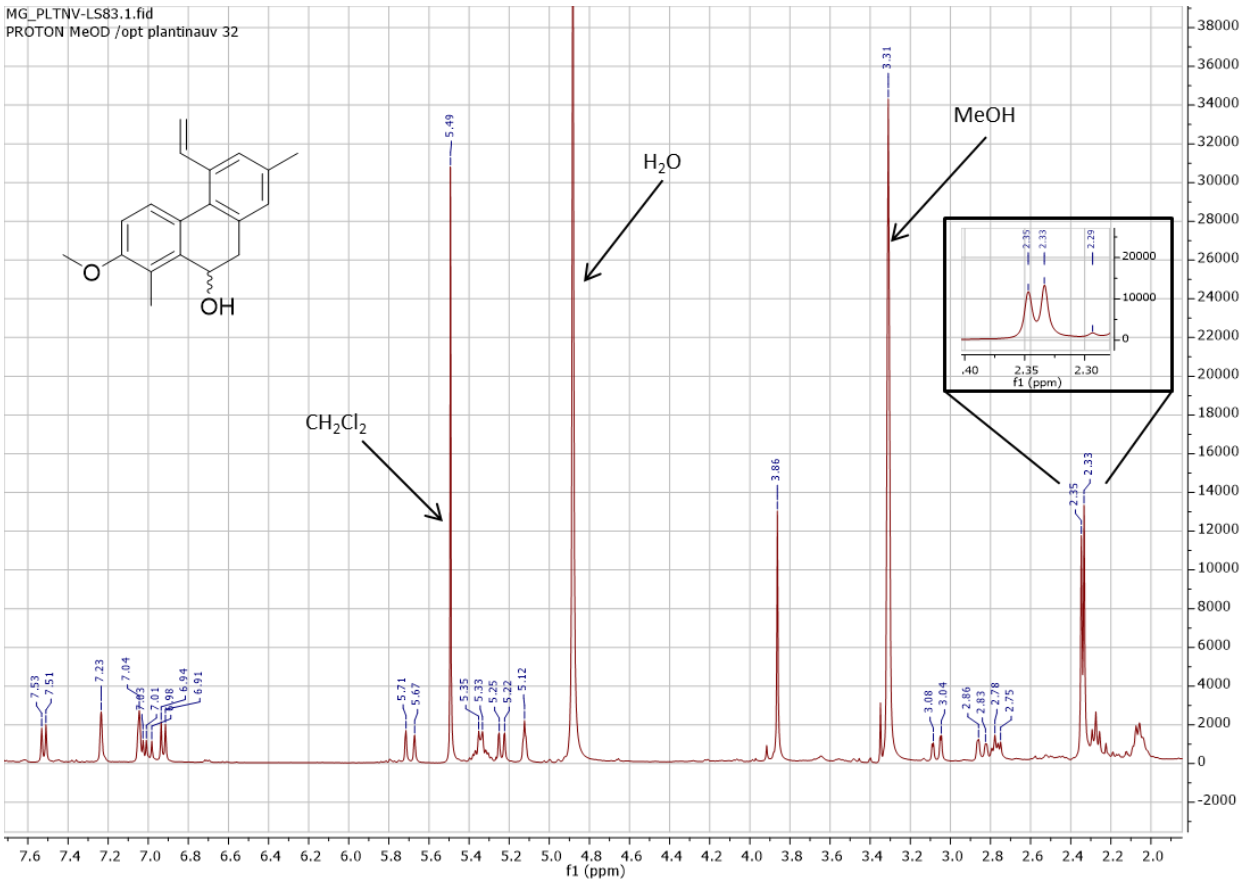

Figure S31. ^{1}H-NMR spectrum of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (8) (500MHz, CD_3OD)

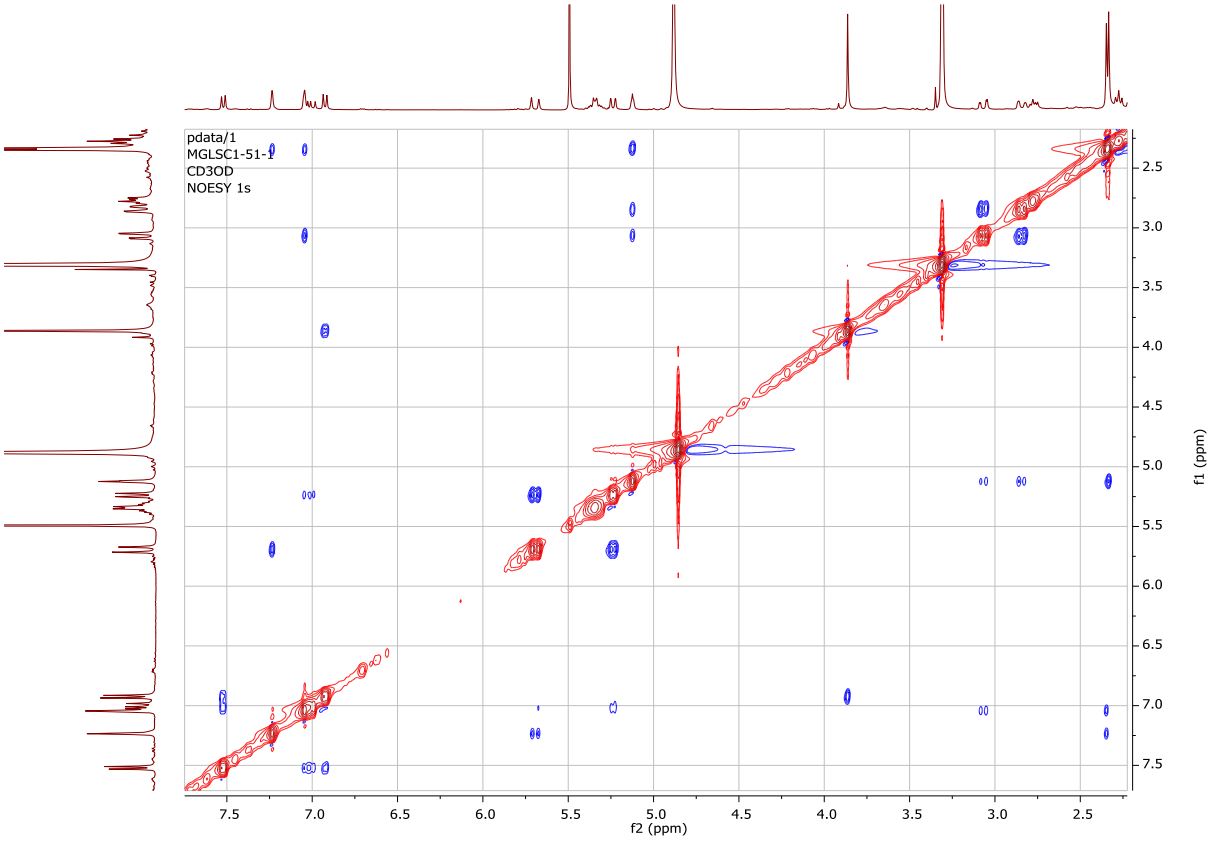

Figure S32. ^{1}H-^{1}H NOESY spectrum of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (8) (400MHz, CD_3OD)

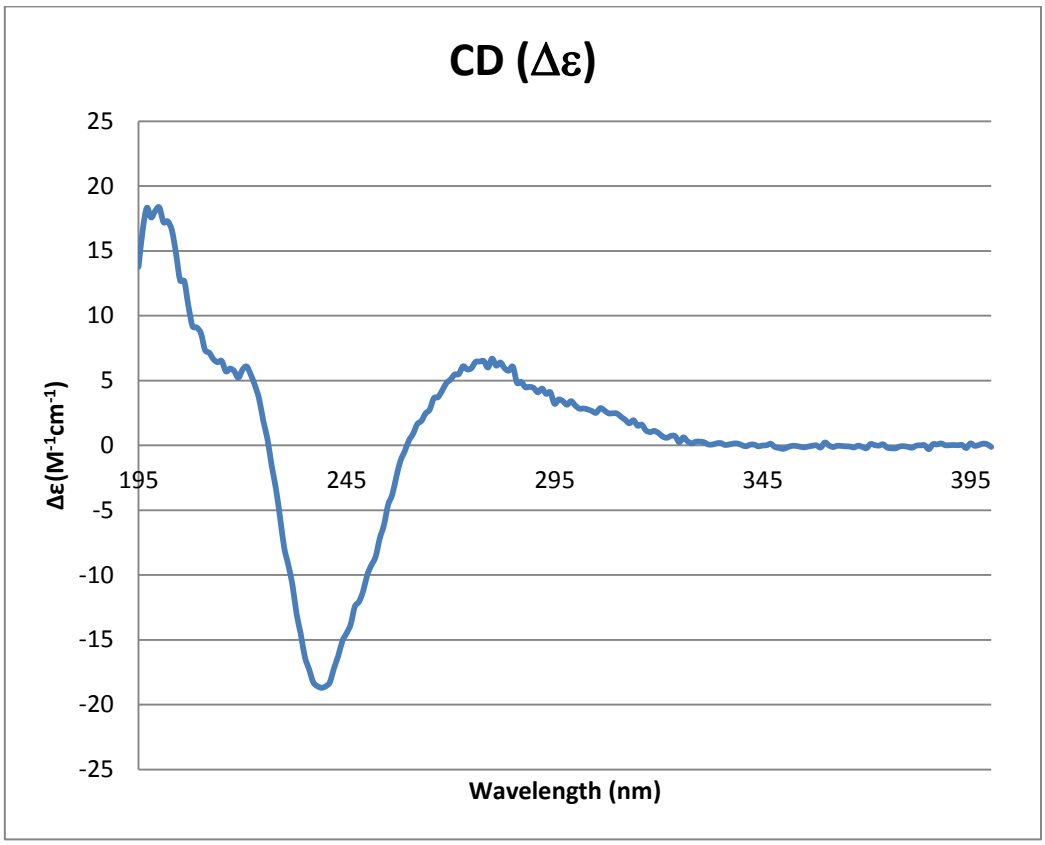

Figure S33. Experimental ECD spectra of compound 8

Circular Dichroism Data Analysis			
Compound:	*Compound 8*	Concentration [M]:	*0,0004*
MW:	500		
Concentration in mg/mL:	0,2	Formula:	[q] = (100 * q)/C*l
Pathlength in cm:	0,1		De = [q]/3298.2
Wavelength (nm)	**CD mdeg (!)**	**Molar ellipticity [θ] (deg cm^2 $dmol^{-1}$)**	**CD (Δε) (mol^{-1} cm^{-1})**
400	-0,163119	-407,7975	-0,123642441
399	0,113959	284,8975	0,086379692
398	0,176983	442,4575	0,134151204
397	0,0305125	76,28125	0,023128146
396	-0,043186	-107,965	-0,032734522
395	0,201054	502,635	0,152396762
394	-0,272805	-682,0125	-0,206783245
393	0,0376598	94,1495	0,028545722
392	0,0113136	28,284	0,008575587

391	0,0335042	83,7605	0,025395822
390	0,0172675	43,16875	0,013088579
389	0,00959835	23,995875	0,007275446
388	0,190505	476,2625	0,144400734
387	0,0958515	239,62875	0,072654402
386	0,121044	302,61	0,091750045
385	-0,388797	-971,9925	-0,294703929
384	0,0141095	35,27375	0,010694849
383	0,00168215	4,205375	0,001275052
382	-0,025767	-64,4175	-0,019531108
381	-0,239674	-599,185	-0,181670305
380	-0,159702	-399,255	-0,121052392
379	-0,0845144	-211,286	-0,064061003
378	-0,114643	-286,6075	-0,086898157
377	-0,301934	-754,835	-0,228862713
376	-0,29269	-731,725	-0,221855861
375	-0,228754	-571,885	-0,173393063
374	0,108948	272,37	0,082581408
373	-0,0282365	-70,59125	-0,021402962
372	0,0268681	67,17025	0,02036573
371	0,134921	337,3025	0,102268662
370	-0,285939	-714,8475	-0,216738676
369	-0,154974	-387,435	-0,117468619
368	-0,0294795	-73,69875	-0,022345143
367	-0,210923	-527,3075	-0,159877357
366	-0,117492	-293,73	-0,089057668
365	-0,0952536	-238,134	-0,072201201
364	-0,061256	-153,14	-0,046431387
363	-0,0375537	-93,88425	-0,028465299
362	-0,167709	-419,2725	-0,127121612
361	-0,0115339	-28,83475	-0,008742572
360	0,295626	739,065	0,224081317
359	-0,218265	-545,6625	-0,165442514
358	0,00193203	4,830075	0,001464458
357	-0,0403899	-100,97475	-0,030615108
356	-0,119997	-299,9925	-0,090956431
355	-0,197973	-494,9325	-0,150061397
354	-0,132357	-330,8925	-0,100325177
353	-0,0485545	-121,38625	-0,036803787
352	-0,0580711	-145,17775	-0,044017267
351	-0,196139	-490,3475	-0,148671245
350	-0,360191	-900,4775	-0,27302089
349	-0,261429	-653,5725	-0,19816036
348	-0,170663	-426,6575	-0,129360712
347	0,165629	414,0725	0,125544994
346	0,0112298	28,0745	0,008512067
345	-0,0119882	-29,9705	-0,009086926
344	-0,0959101	-239,77525	-0,072698821

343	0,0758133	189,53325	0,057465663
342	0,0616317	154,07925	0,046716163
341	-0,0982898	-245,7245	-0,074502607
340	0,0347702	86,9255	0,026355436
339	0,180514	451,285	0,136827664
338	0,182117	455,2925	0,13804272
337	0,092337	230,8425	0,069990449
336	0,0403143	100,78575	0,030557804
335	0,230242	575,605	0,174520951
334	0,204752	511,88	0,155199806
333	0,0879622	219,9055	0,066674398
332	0,0873766	218,4415	0,06623052
331	0,30962	774,05	0,234688618
330	0,376706	941,765	0,285539082
329	0,370335	925,8375	0,280709933
328	0,19714	492,85	0,149429992
327	0,403825	1009,5625	0,306094991
326	0,817276	2043,19	0,619486387
325	0,31799	794,975	0,241032988
324	0,936611	2341,5275	0,709941028
323	0,966358	2415,895	0,732488933
322	0,766985	1917,4625	0,581366351
321	0,900962	2252,405	0,682919471
320	1,25257	3131,425	0,94943454
319	1,46974	3674,35	1,114047056
318	1,35443	3386,075	1,026643321
317	1,51093	3777,325	1,145268631
316	2,1112	5278	1,600266812
315	1,99186	4979,65	1,50980838
314	2,55771	6394,275	1,938716573
313	2,23978	5599,45	1,697729064
312	2,60288	6507,2	1,972954945
311	2,90215	7255,375	2,199798375
310	3,24893	8122,325	2,462653872
309	3,26255	8156,375	2,472977685
308	3,25726	8143,15	2,468967922
307	3,55347	8883,675	2,693491905
306	3,79064	9476,6	2,873264205
305	3,30769	8269,225	2,507193318
304	3,49303	8732,575	2,647679037
303	3,65719	9142,975	2,772110545
302	3,75378	9384,45	2,845324723
301	3,73557	9338,925	2,831521739
300	4,04728	10118,2	3,067794555
299	4,49757	11243,925	3,409109514
298	4,1346	10336,5	3,133982172
297	4,50355	11258,875	3,41364229
296	4,66739	11668,475	3,537831241

295	4,23045	10576,125	3,206635438
294	5,40447	13511,175	4,096529925
293	5,2372	13093	3,969741071
292	5,77874	14446,85	4,380222546
291	5,3931	13482,75	4,087911588
290	5,83668	14591,7	4,42414044
289	5,95453	14886,325	4,513469468
288	5,91351	14783,775	4,482376751
287	6,46694	16167,35	4,901870717
286	6,35853	15896,325	4,819697108
285	8,00074	20001,85	6,064474562
284	7,59444	18986,1	5,756503547
283	7,84919	19622,975	5,949601298
282	8,43413	21085,325	6,392979504
281	8,11056	20276,4	6,147716937
280	8,82744	22068,6	6,691104239
279	7,91855	19796,375	6,002175429
278	8,57804	21445,1	6,502061731
277	8,52826	21320,65	6,464329028
276	8,48301	21207,525	6,430030016
275	7,84431	19610,775	5,94590231
274	7,73147	19328,675	5,860370808
273	8,0453	20113,25	6,098250561
272	7,25386	18134,65	5,498347584
271	7,21191	18029,775	5,466549936
270	6,69367	16734,175	5,07372961
269	6,32994	15824,85	4,798026196
268	5,57663	13941,575	4,227025347
267	4,89786	12244,65	3,712525014
266	4,80467	12011,675	3,641888
265	3,64094	9102,35	2,759793221
264	3,24267	8106,675	2,457908859
263	2,48478	6211,95	1,88343642
262	2,15737	5393,425	1,635263174
261	1,1748	2937	0,890485719
260	0,493709	1234,2725	0,374226093
259	-0,595266	-1488,165	-0,451205203
258	-1,53945	-3848,625	-1,166886484
257	-3,16377	-7909,425	-2,398103511
256	-5,01369	-12534,225	-3,800322903
255	-6,05618	-15140,45	-4,590519071
254	-8,11801	-20295,025	-6,153363956
253	-9,46223	-23655,575	-7,172268207
252	-11,3297	-28324,25	-8,58779031
251	-12,177	-30442,5	-9,230034564
250	-13,165	-32912,5	-9,9789279
249	-14,835	-37087,5	-11,24476987
248	-15,918	-39795	-12,06567218

247	-16,3988	-40997	-12,4301134
246	-18,2236	-45559	-13,8132921
245	-19,1244	-47811	-14,49608878
244	-19,9221	-49805,25	-15,10073677
243	-21,4392	-53598	-16,25068219
242	-22,6685	-56671,25	-17,18247832
241	-24,0986	-60246,5	-18,26647869
240	-24,5171	-61292,75	-18,58369717
239	-24,6689	-61672,25	-18,69875993
238	-24,5026	-61256,5	-18,57270632
237	-24,0983	-60245,75	-18,26625129
236	-22,777	-56942,5	-17,26472015
235	-21,5548	-53887	-16,33830574
234	-19,1994	-47998,5	-14,55293797
233	-17,1687	-42921,75	-13,01368929
232	-14,1935	-35483,75	-10,7585198
231	-12,1725	-30431,25	-9,226623613
230	-10,3688	-25922	-7,859438482
229	-7,2589	-18147,25	-5,502167849
228	-4,32955	-10823,875	-3,281752168
227	-2,05302	-5132,55	-1,556167
226	0,625187	1562,9675	0,473884998
225	2,47556	6188,9	1,876447759
224	4,70458	11761,45	3,56602086
223	6,08915	15222,875	4,615509975
222	7,17644	17941,1	5,439664059
221	8,02516	20062,9	6,082984658
220	7,70398	19259,95	5,839533685
219	6,87114	17177,85	5,208249955
218	7,54663	18866,575	5,720264083
217	7,81175	19529,375	5,921222182
216	7,52711	18817,775	5,705468134
215	8,58697	21467,425	6,508830574
214	8,45725	21143,125	6,410504214
213	8,76681	21917,025	6,645147353
212	9,42808	23570,2	7,146382876
211	9,68364	24209,1	7,340094597
210	11,4029	28507,25	8,64327512
209	12,0003	30000,75	9,096097872
208	12,1007	30251,75	9,172199988
207	14,1605	35401,25	10,73350615
206	16,7203	41800,75	12,67380692
205	16,7735	41933,75	12,71413195
204	19,5621	48905,25	14,82786065
203	21,9164	54791	16,61239464
202	22,7995	56998,75	17,28177491
201	22,7036	56759	17,20908374
200	24,2078	60519,5	18,34925111

199	23,8393	59598,25	18,06993208
198	23,1784	57946	17,56897702
197	24,1677	60419,25	18,31885574
196	21,9197	54799,25	16,614896
195	18,1726	45431,5	13,77463465

Table 1. EDC data

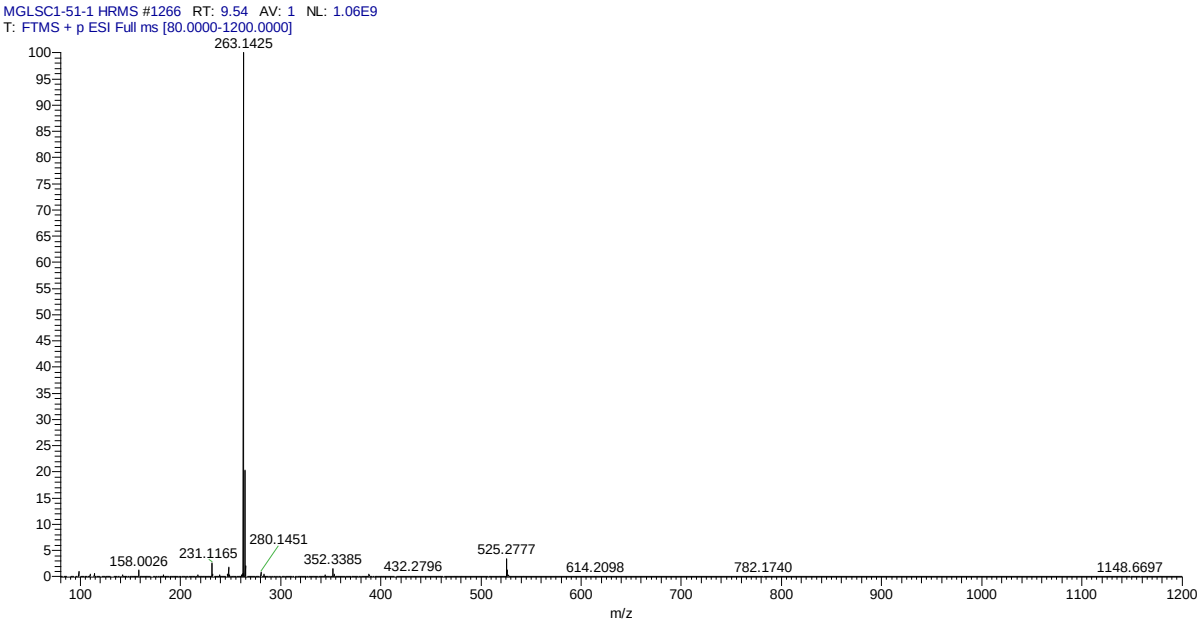

Figure S34. HRESIMS of 2-methoxy-1,7-dimethyl-5-vinyl-9,10-dihydrophenanthren-10-ol (**8**) (positive ionisation mode)

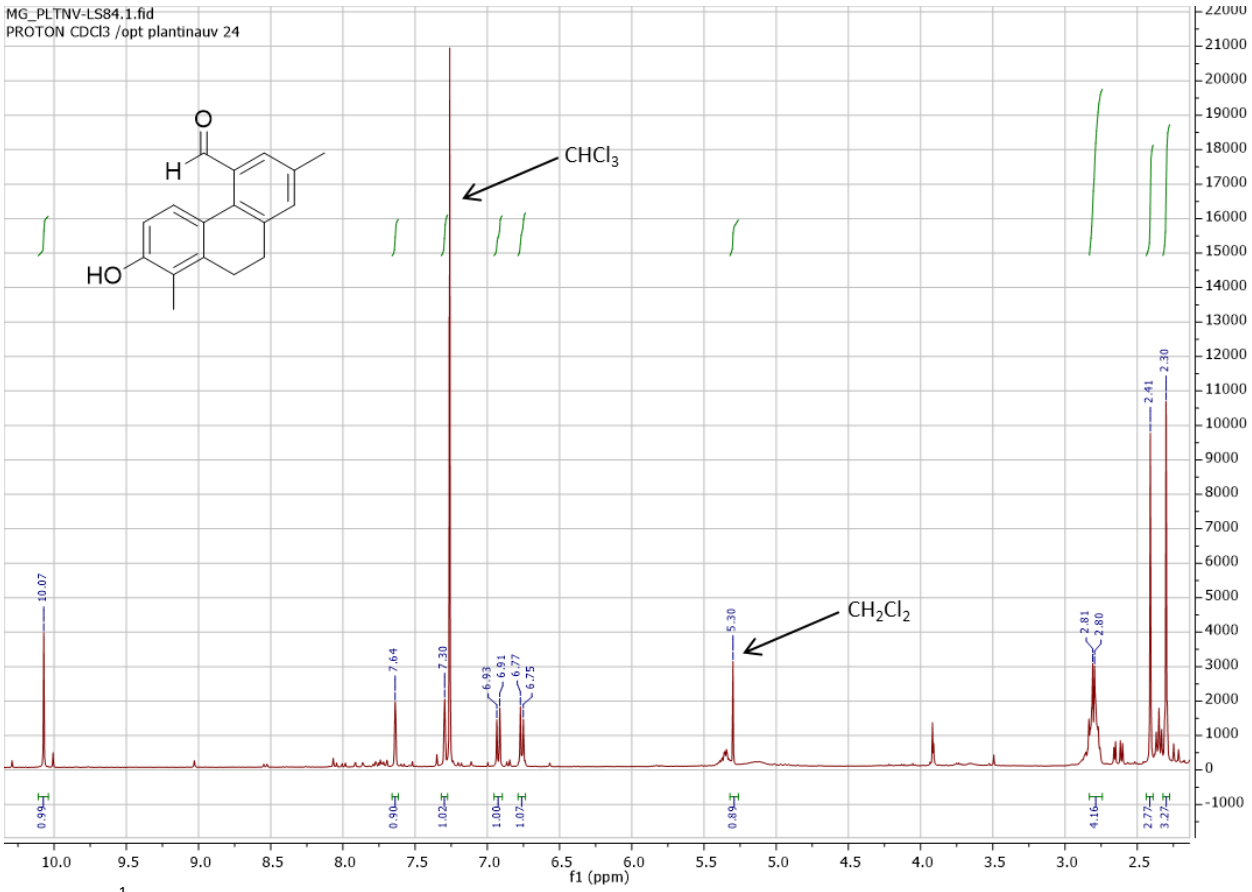

Figure S35. ^{1}H-NMR spectrum of 2-hydroxy-1,7-dimethyl-9,10-dihydrophenanthrene-5-carbaldehyde (**9**) (400MHz, $CDCl_3$)

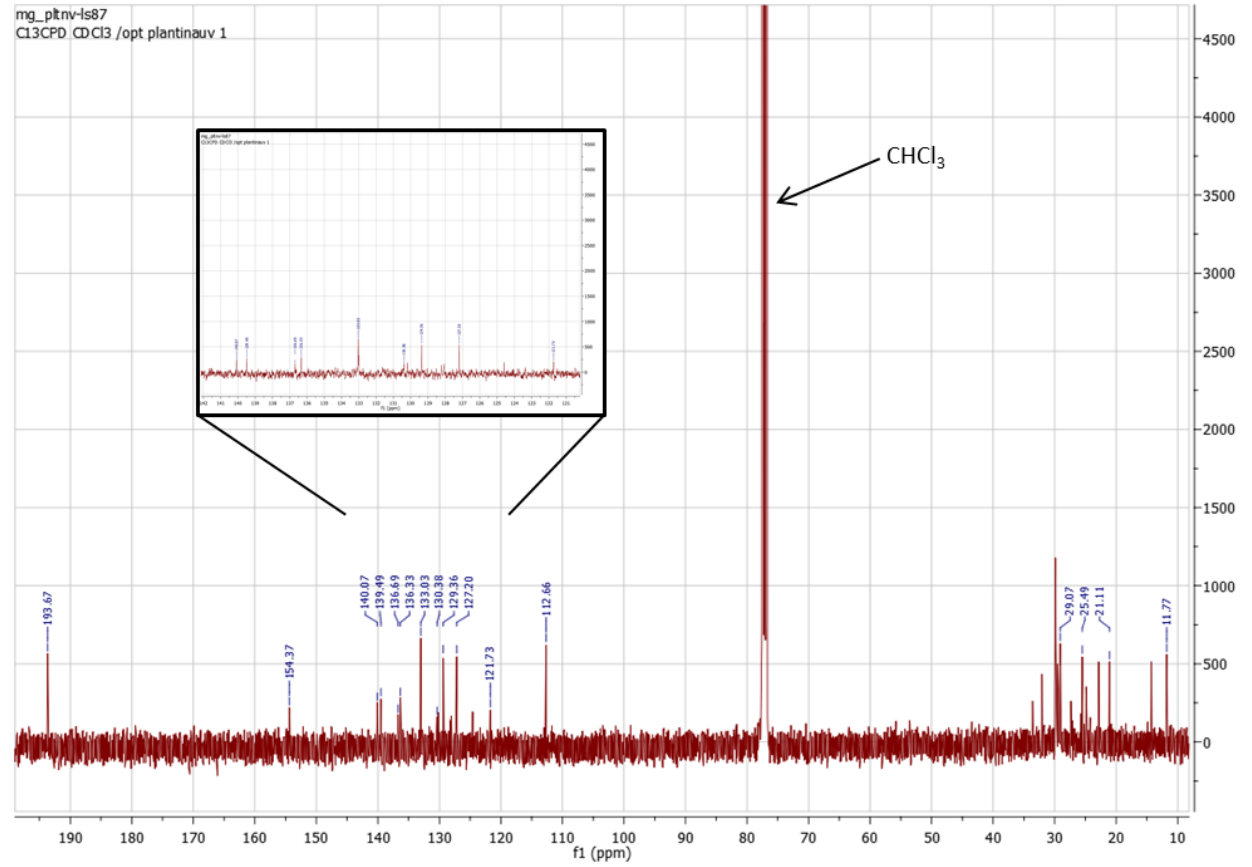

Figure S36. ^{13}C-NMR spectrum of 2-hydroxy-1,7-dimethyl-9,10-dihydrophenanthrene-5-carbaldehyde (**9**) (100MHz, $CDCl_3$)

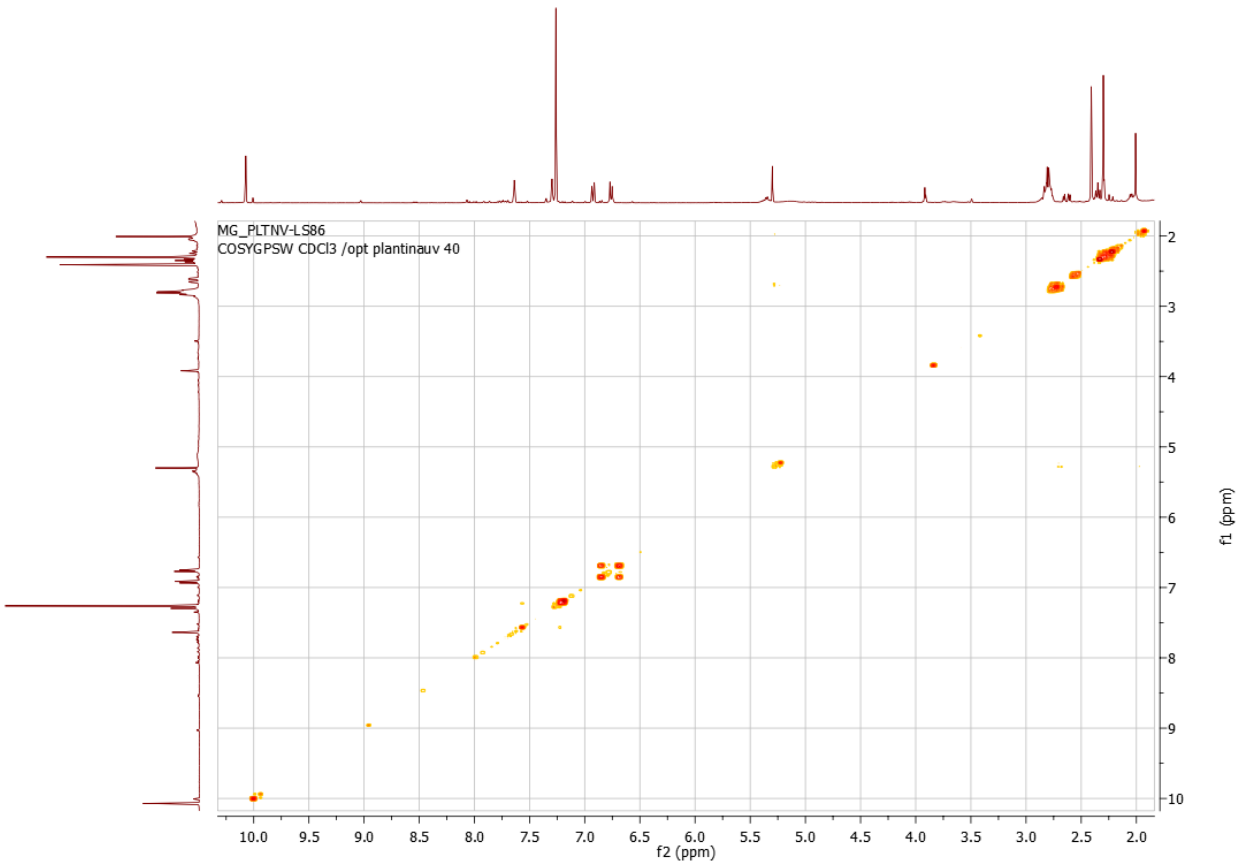

Figure S37. ^{1}H-^{1}H COSY spectrum of 2-hydroxy-1,7-dimethyl-9,10-dihydrophenanthrene-5-carbaldehyde (**9**) (400MHz, $CDCl_3$)

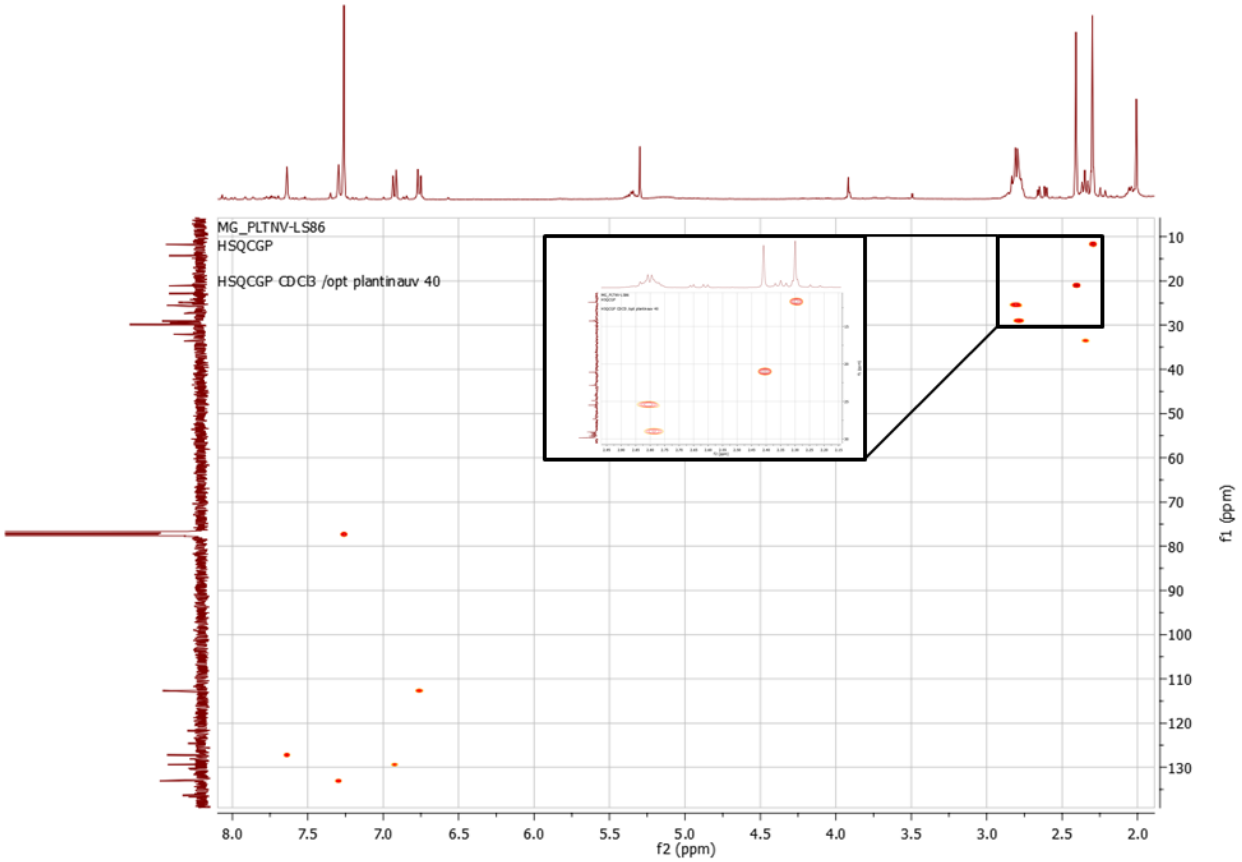

Figure S38. ^{1}H-^{13}C HSQC spectrum of 2-hydroxy-1,7-dimethyl-9,10-dihydrophenanthrene-5-carbaldehyde (**9**) (400MHz, $CDCl_3$)

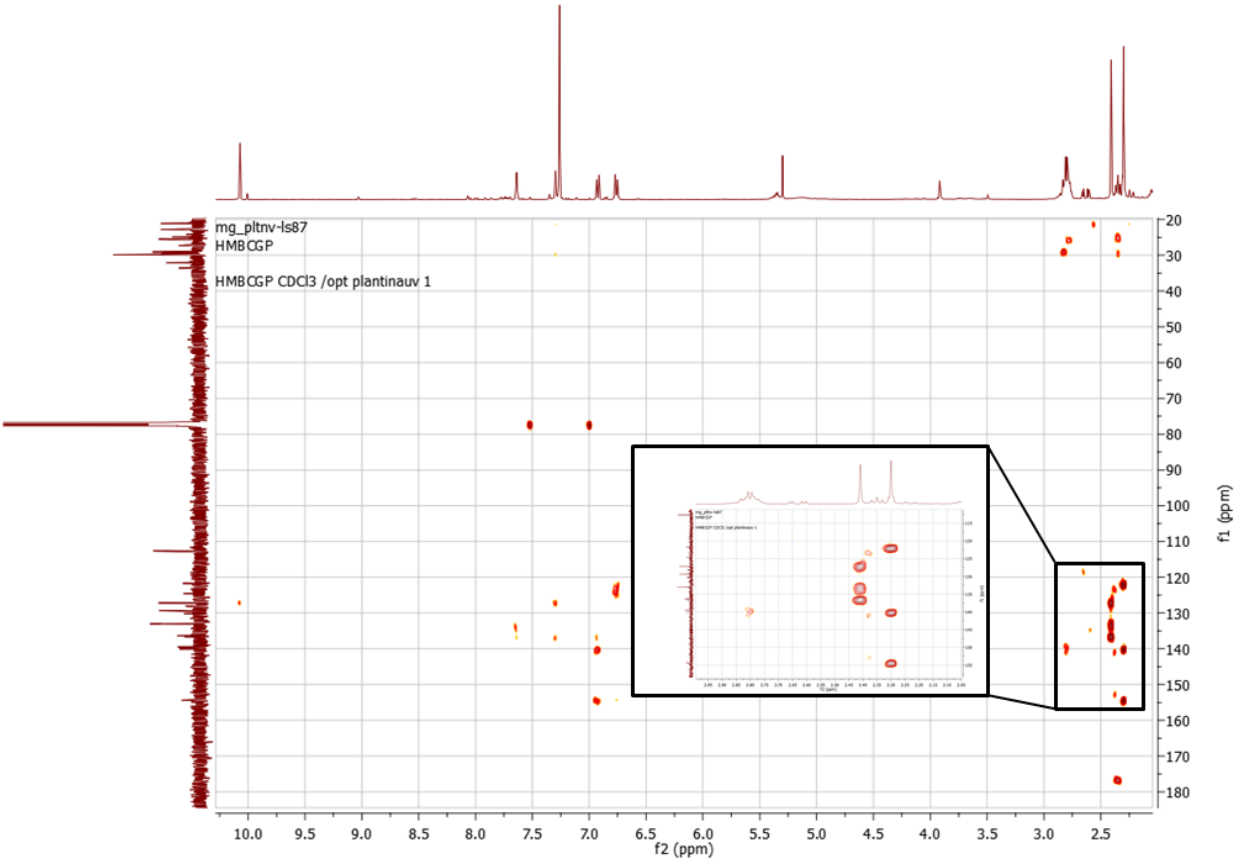

Figure S39. ^{1}H-^{13}C HMBC spectrum of 2-hydroxy-1,7-dimethyl-9,10-dihydrophenanthrene-5-carbaldehyde (**9**) (400MHz, $CDCl_3$)

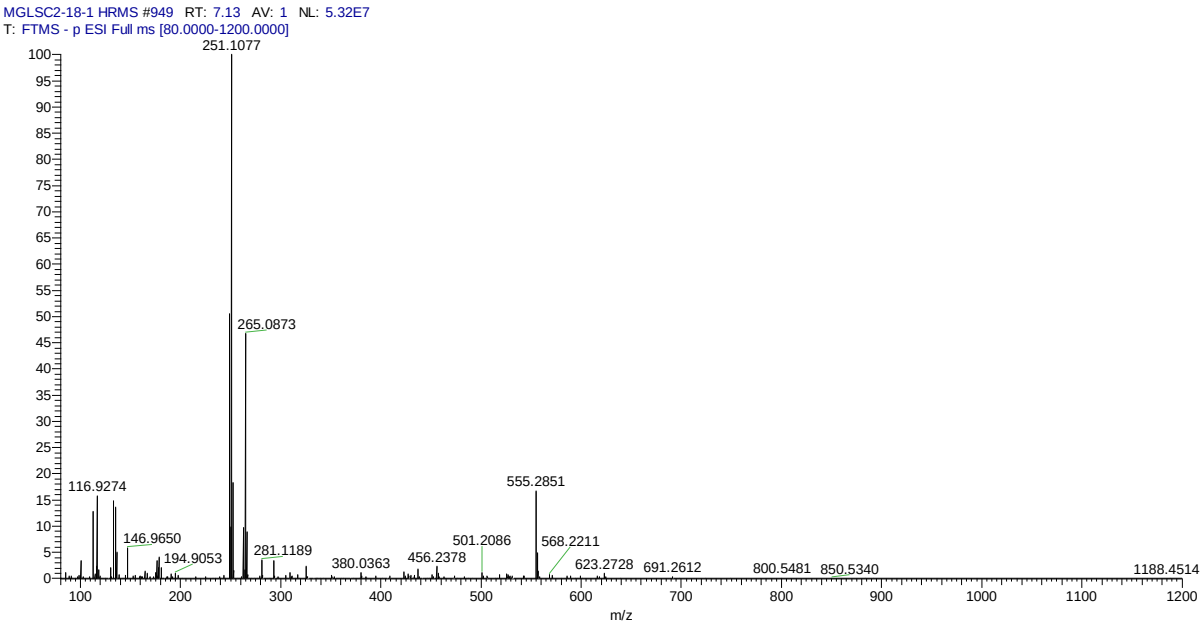

Figure S40. HRESIMS of 2-hydroxy-1,7-dimethyl-9,10-dihydrophenanthrene-5-carbaldehyde (**9**) (negative ionisation mode)