

Communication

A New Pyrrole Alkaloid from *Capsicum annuum* L. var. Palmera Grown in La Palma (Canary Islands, Spain)

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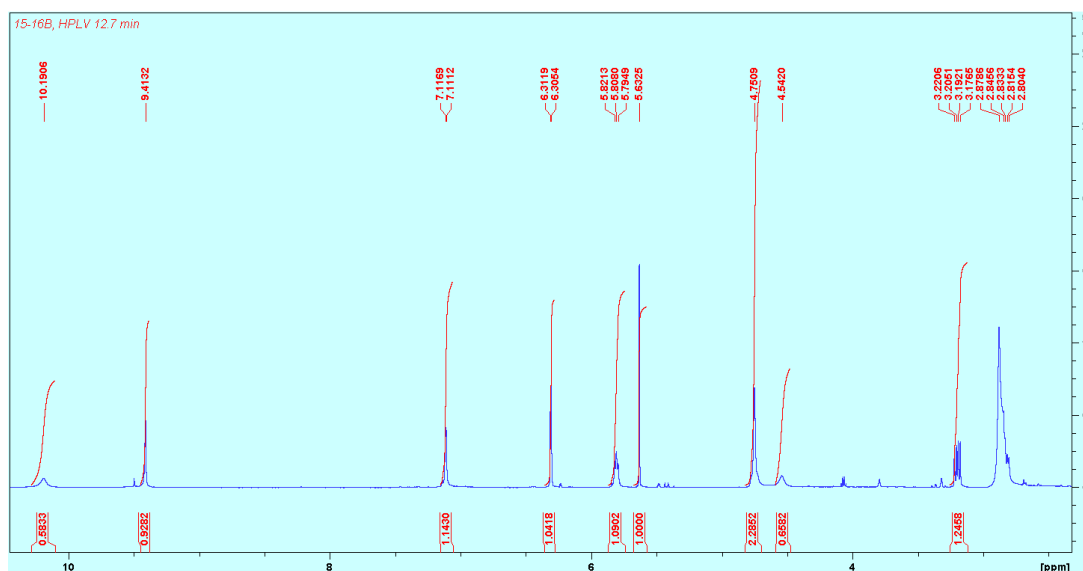


Figure S1. ¹H NMR spectrum of compound **8** (acetone-*d*₆).

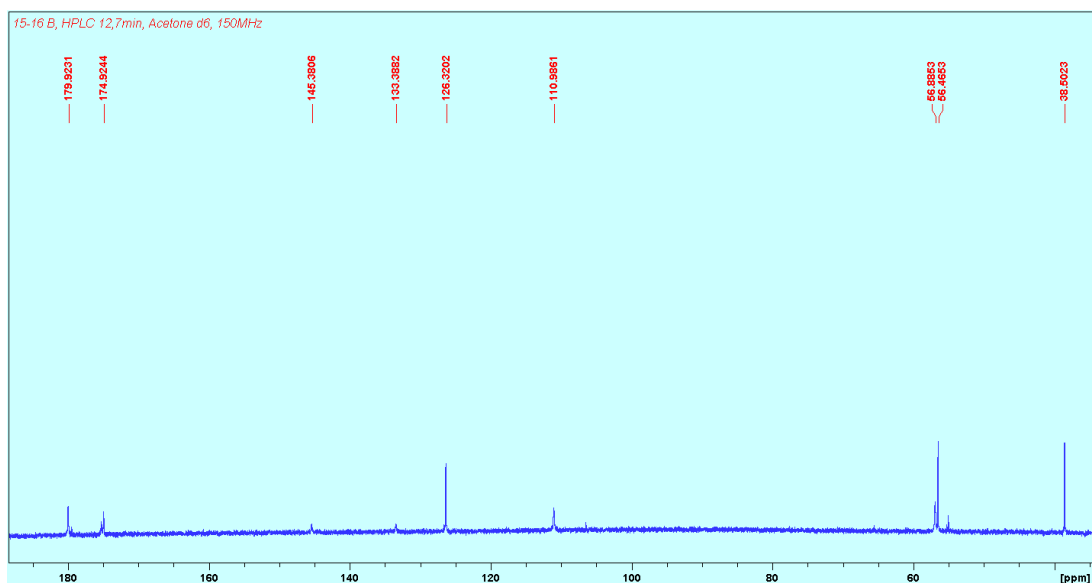


Figure S2. ^{13}C NMR spectrum of compound **8** (acetone- d_6)

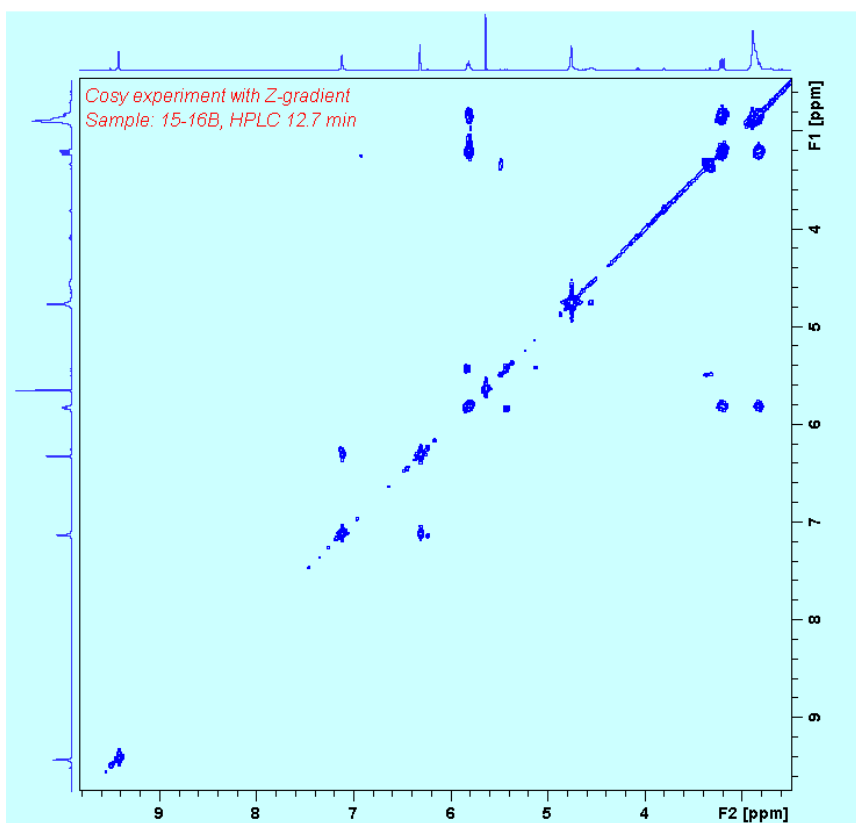


Figure S3. COSY spectrum of compound **8** (acetone- d_6)

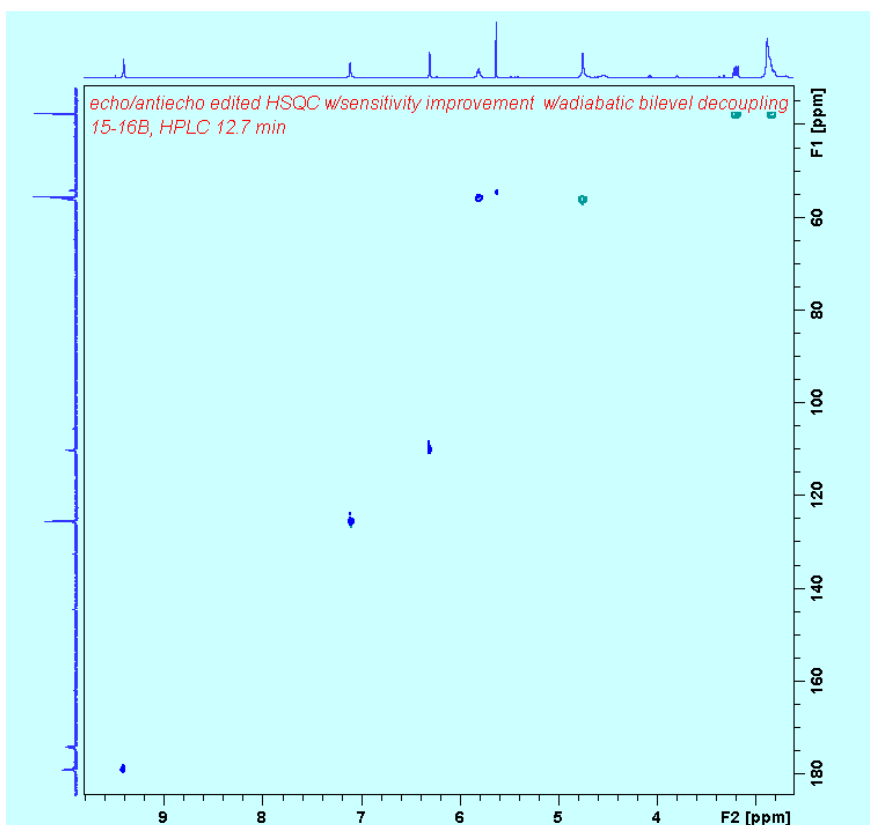


Figure S4. HSQC spectrum of compound **8** (acetone-*d*₆)

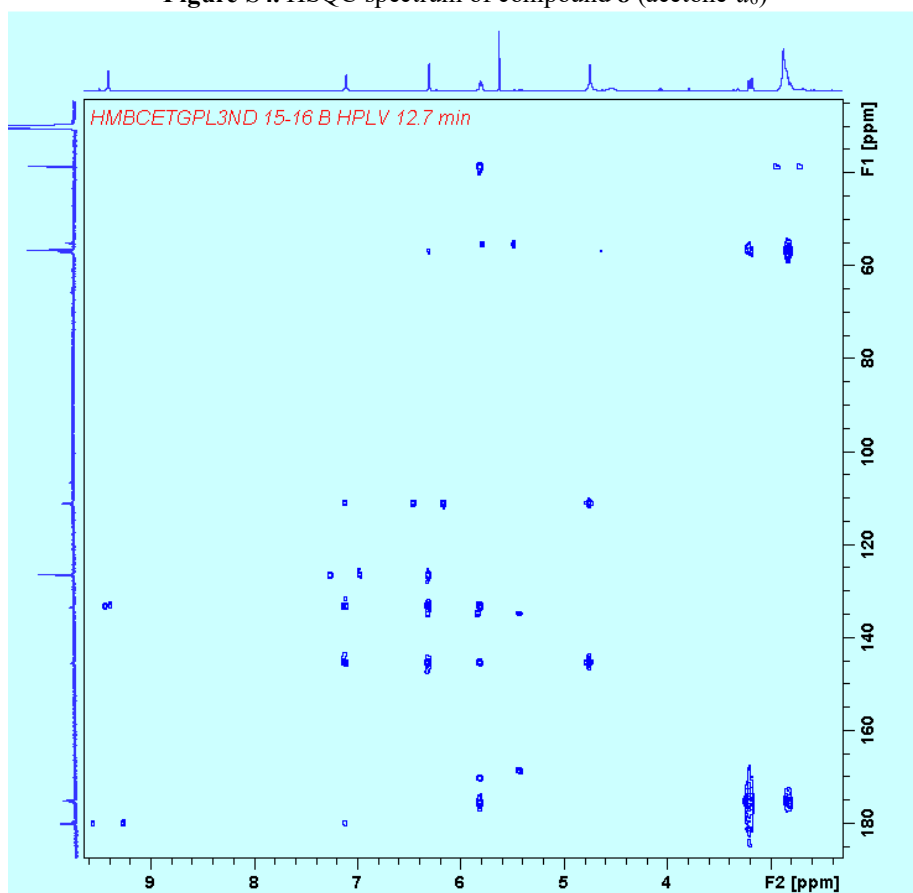


Figure S5. HMBC spectrum of compound **8** (acetone-*d*₆)

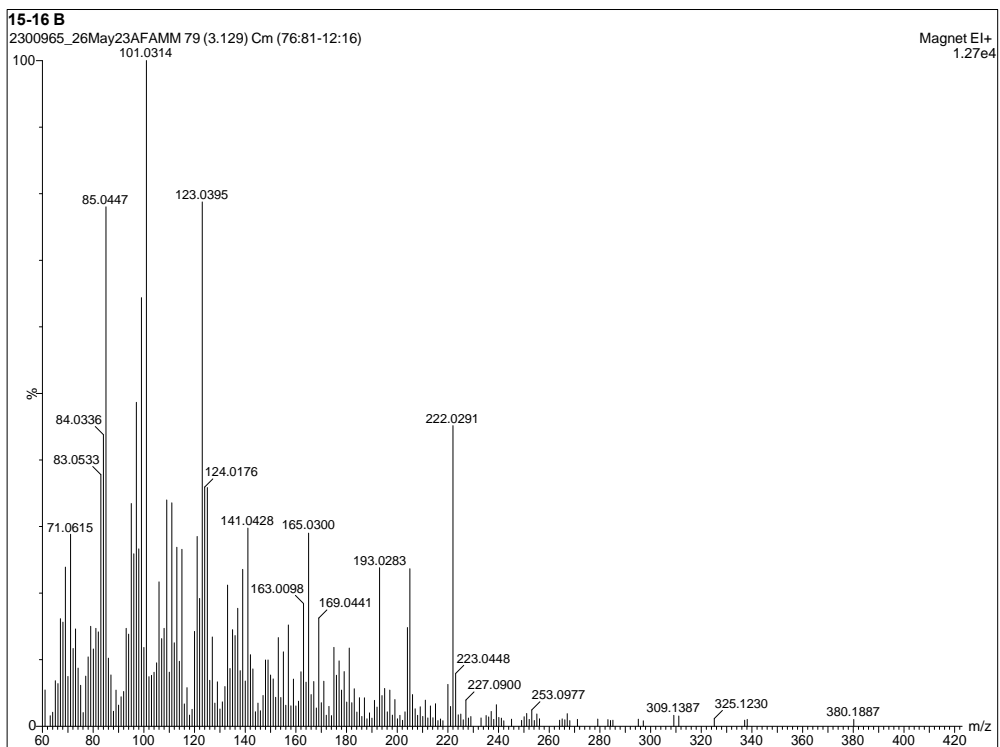


Figure S6. HREIMS spectrum of compound 8

Multiple Mass Analysis: 13179 mass(es) processed - displaying only valid results

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

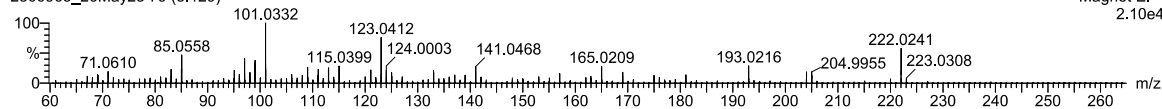
127124 formula(e) evaluated with 131 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 10-10 H: 5-10 N: 0-1 O: 0-5

15-16 B

2300965_26May23 79 (3,129)

Magnet EI+
2.10e4

Minimum: 0.10
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
224.0565	0.29	224.0559	0.6	2.7	6.5	C10 H10 N O5
224.0545	0.20	224.0559	-1.4	-6.2	6.5	C10 H10 N O5
223.0493	0.51	223.0481	1.2	5.4	7.0	C10 H9 N O5
223.0472	0.55	223.0481	-0.9	-4.0	7.0	C10 H9 N O5
222.0405	1.48	222.0402	0.3	1.4	7.5	C10 H8 N O5
222.0384	3.37	222.0402	-1.8	-8.1	7.5	C10 H8 N O5
221.0341	0.31	221.0324	1.7	7.7	8.0	C10 H7 N O5
221.0321	0.30	221.0324	-0.3	-1.4	8.0	C10 H7 N O5
220.0263	0.26	220.0246	1.7	7.7	8.5	C10 H6 N O5
220.0243	0.37	220.0246	-0.3	-1.4	8.5	C10 H6 N O5
219.0170	0.15	219.0168	0.2	0.9	9.0	C10 H5 N O5
219.0150	0.15	219.0168	-1.8	-8.2	9.0	C10 H5 N O5
210.0543	0.16	210.0528	1.5	7.1	6.0	C10 H10 O5
210.0523	0.23	210.0528	-0.5	-2.4	6.0	C10 H10 O5
209.0465	0.17	209.0450	1.5	7.2	6.5	C10 H9 O5
208.0627	0.59	208.0610	1.7	8.2	6.5	C10 H10 N O4
208.0607	0.67	208.0610	-0.3	-1.4	6.5	C10 H10 N O4
208.0378	0.13	208.0372	0.6	2.9	7.0	C10 H8 O5
208.0358	0.12	208.0372	-1.4	-6.7	7.0	C10 H8 O5
207.0549	0.42	207.0532	1.7	8.2	7.0	C10 H9 N O4
207.0530	0.32	207.0532	-0.2	-1.0	7.0	C10 H9 N O4
207.0511	0.38	207.0532	-2.1	-10.1	7.0	C10 H9 N O4
207.0301	0.37	207.0293	0.8	3.9	7.5	C10 H7 O5
207.0282	0.39	207.0293	-1.1	-5.3	7.5	C10 H7 O5
206.0463	0.17	206.0453	1.0	4.9	7.5	C10 H8 N O4
206.0444	0.19	206.0453	-0.9	-4.4	7.5	C10 H8 N O4
206.0235	1.62	206.0215	2.0	9.7	8.0	C10 H6 O5
206.0217	1.61	206.0215	0.2	1.0	8.0	C10 H6 O5
206.0198	1.63	206.0215	-1.7	-8.3	8.0	C10 H6 O5
205.0389	0.23	205.0375	1.4	6.8	8.0	C10 H7 N O4
205.0370	0.42	205.0375	-0.5	-2.4	8.0	C10 H7 N O4
205.0144	9.68	205.0137	0.7	3.4	8.5	C10 H5 O5
205.0125	7.77	205.0137	-1.2	-5.9	8.5	C10 H5 O5
204.0308	0.26	204.0297	1.1	5.4	8.5	C10 H6 N O4
204.0289	0.31	204.0297	-0.8	-3.9	8.5	C10 H6 N O4
203.0238	0.23	203.0219	1.9	9.4	9.0	C10 H5 N O4
203.0220	0.24	203.0219	0.1	0.5	9.0	C10 H5 N O4
203.0201	0.25	203.0219	-1.8	-8.9	9.0	C10 H5 N O4
194.0592	0.30	194.0579	1.3	6.7	6.0	C10 H10 O4
194.0574	0.49	194.0579	-0.5	-2.6	6.0	C10 H10 O4
193.0518	0.59	193.0501	1.7	8.8	6.5	C10 H9 O4
193.0500	0.65	193.0501	-0.1	-0.5	6.5	C10 H9 O4
193.0482	0.87	193.0501	-1.9	-9.8	6.5	C10 H9 O4
192.0673	0.48	192.0661	1.2	6.2	6.5	C10 H10 N O3
192.0655	0.43	192.0661	-0.6	-3.1	6.5	C10 H10 N O3
192.0425	0.14	192.0423	0.2	1.0	7.0	C10 H8 O4
192.0408	0.12	192.0423	-1.5	-7.8	7.0	C10 H8 O4
191.0597	0.61	191.0582	1.5	7.9	7.0	C10 H9 N O3
191.0579	0.52	191.0582	-0.3	-1.6	7.0	C10 H9 N O3
191.0350	0.27	191.0344	0.6	3.1	7.5	C10 H7 O4
191.0332	0.23	191.0344	-1.2	-6.3	7.5	C10 H7 O4
190.0521	0.17	190.0504	1.7	8.9	7.5	C10 H8 N O3
190.0503	0.12	190.0504	-0.1	-0.5	7.5	C10 H8 N O3
190.0486	0.13	190.0504	-1.8	-9.5	7.5	C10 H8 N O3

Figure S7. Elemental analysis of compound 8

Elemental Composition Report

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass. Even Electron Ions

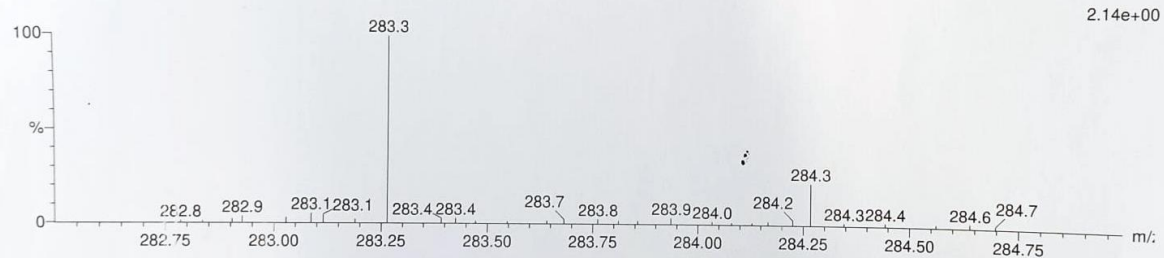
1452 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-40 N: 0-3 O: 0-10 Na: 0-2 Si: 0-1

20230609-LCT 71-73D Neg 5 (0.227)

1: TOF MS ES-



Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
283.2640	100.00	283.2637	0.3	1.1	1.5	68.8	0.0	C18 H35 O2
284.2669	22.17	284.2678	-0.9	-3.2	-1.5	29.8	0.0	C14 H35 N3 O Na

Figure S8. TOF MS ES- spectrum corresponding to compound **6** (Fractions 71-73D).