

Accelerating the Discovery of Biologically Active Small Molecules

Using a High-Throughput Yeast Halo Assay[#]

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[#] Dedicated to the late Dr. Kenneth L. Rinehart of the University of Illinois at Urbana-Champaign for his pioneering work on bioactive natural products.

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Figure S1: Above Water (A) and Below Water (B) Images of *Monanchora unguifera*, UCSC Collection Number 03500.

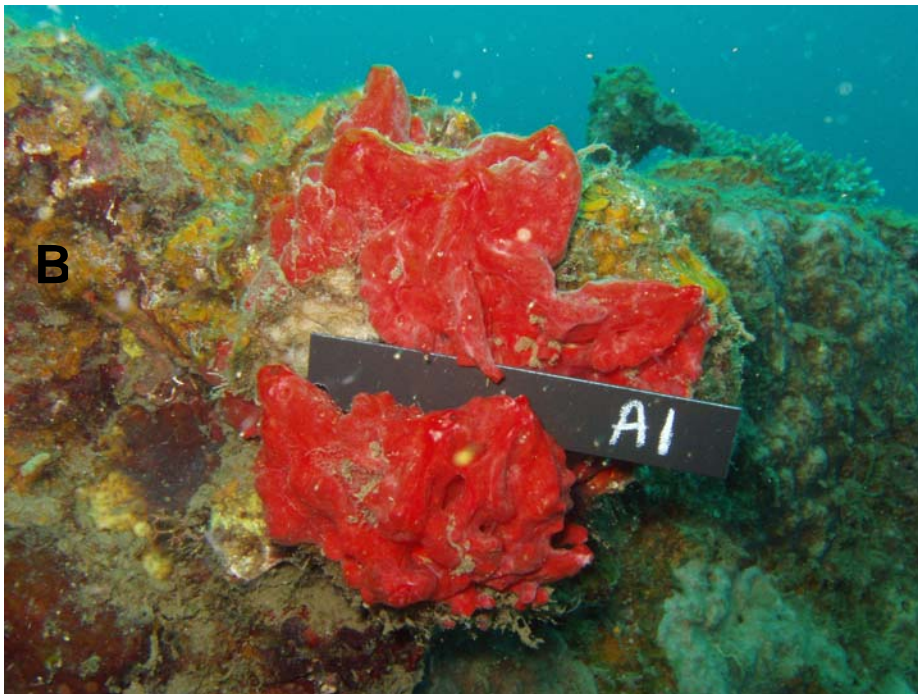
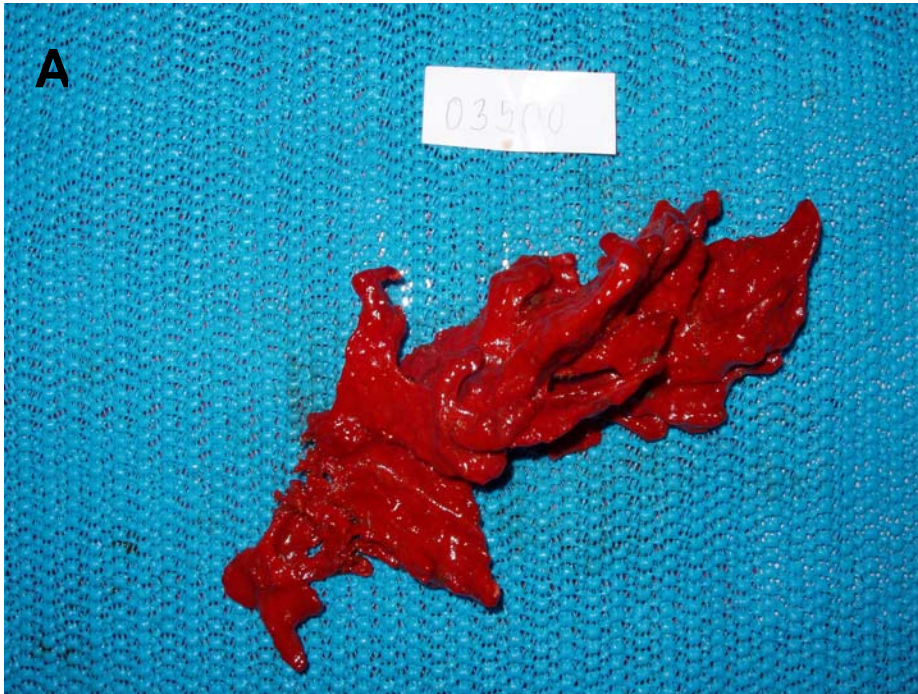


Figure S2: Isolation Scheme for Crambescidin 800.

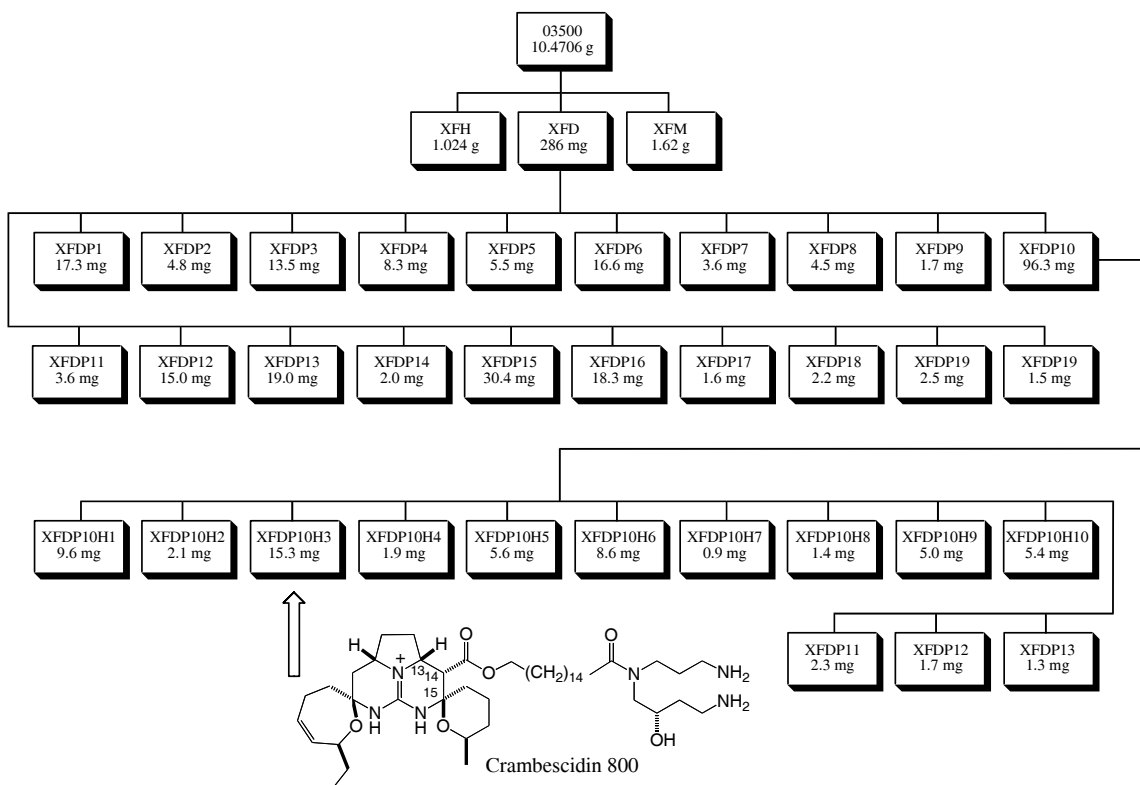


Figure S3: ^1H NMR Spectrum of Crambescidin 800.

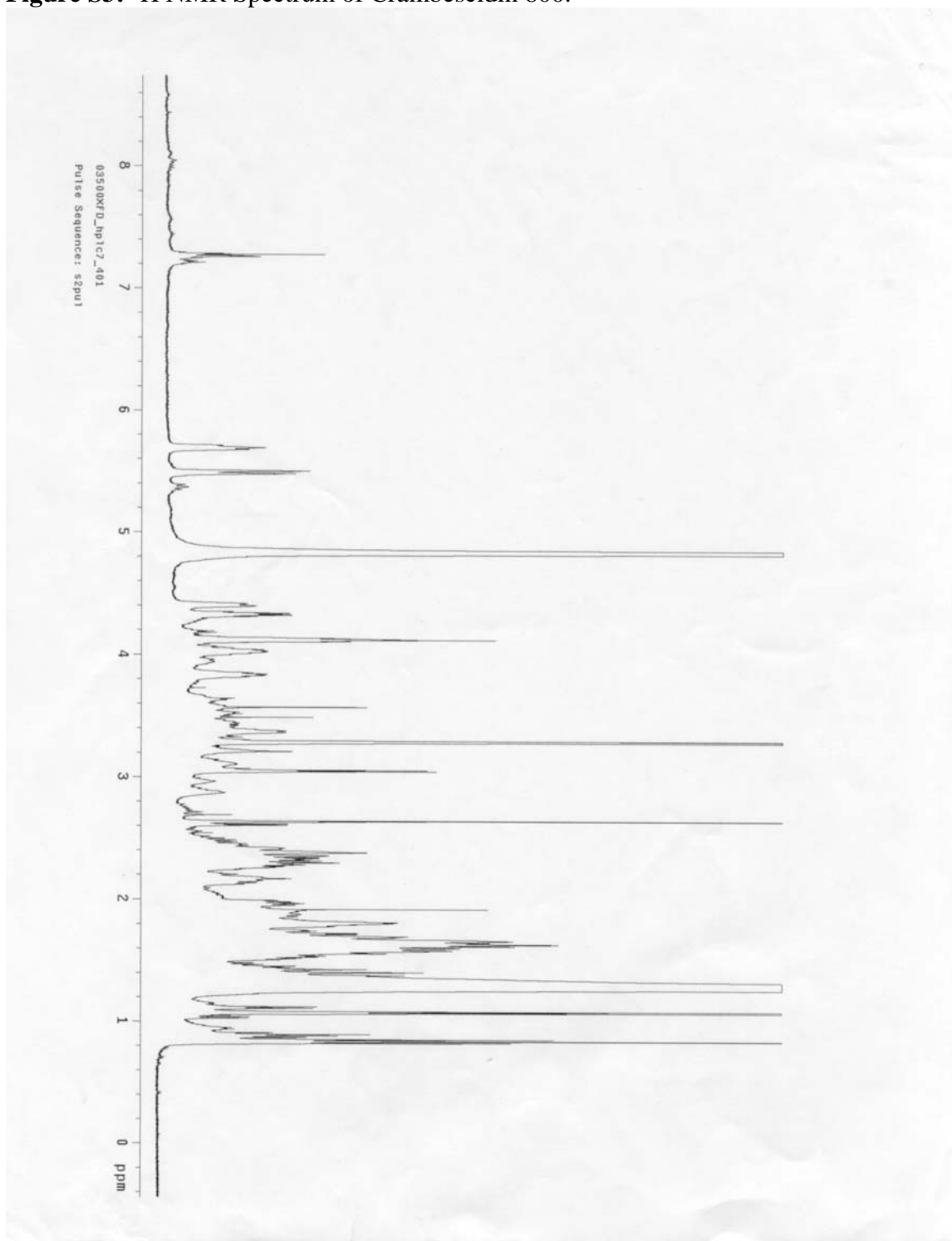


Figure S4: ^{13}C NMR Spectrum of Crambescidin 800.

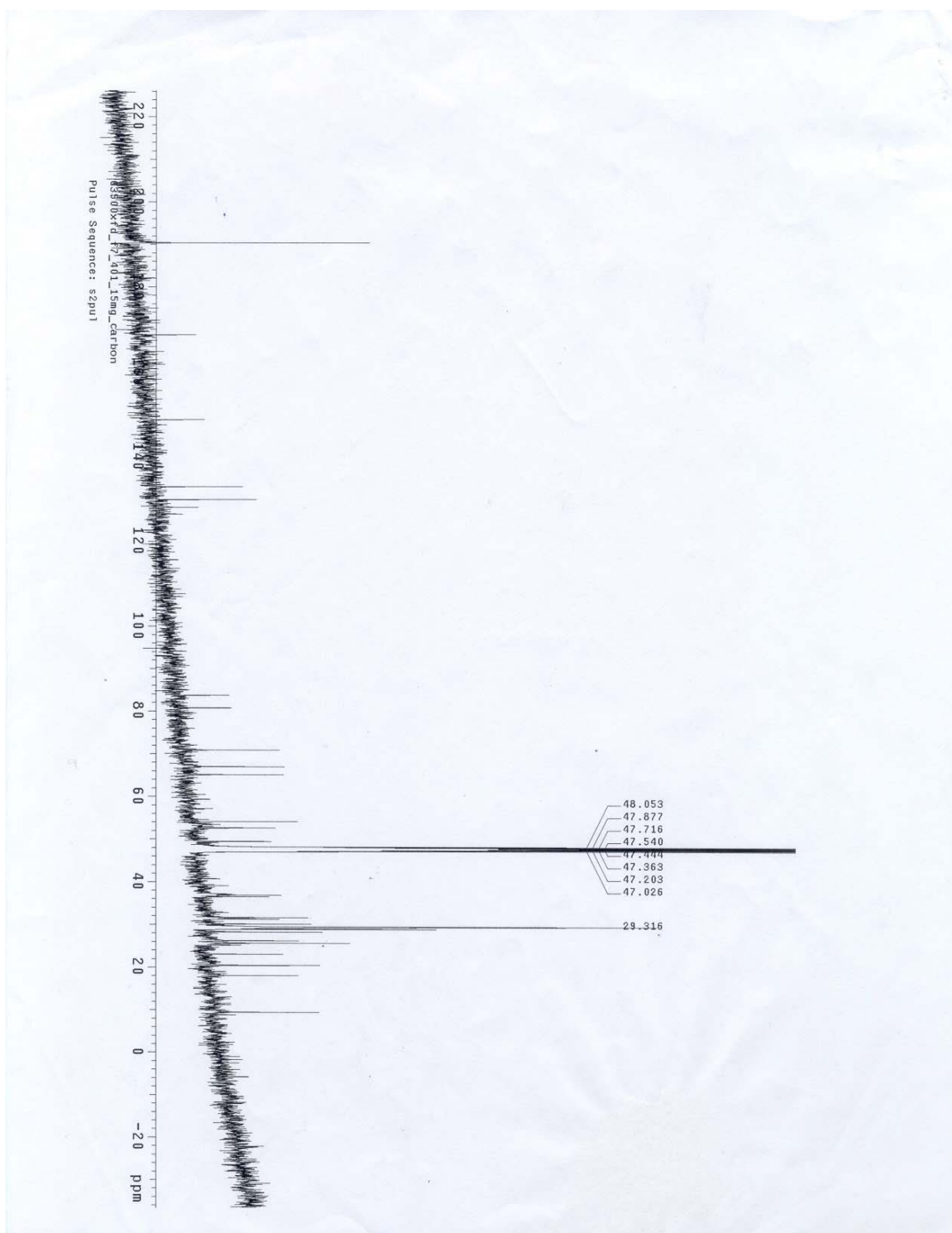
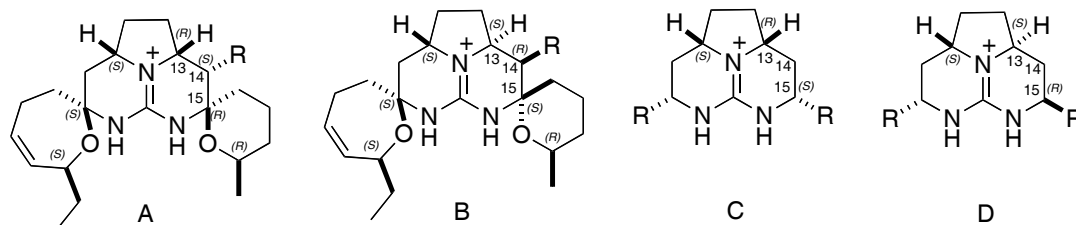


Table S1. Comparison of ^{13}C NMR Signals for Several Known Polycyclic Guanidinium Alkaloids.

	crambescidin 800 CD_3OD	acetylcrambescidin 800 CDCl_3	ptilomycalin A CDCl_3	13,14,15-isocrambescidin 800 CD_3OD	experimental CD_3OD
C-1	9.4	10.1	10.2	10.7	10.9
C-2	26.2	29.8	29.2	30.2	29.8
C-3	72.2	71.0	70.9	71.9	71.9
C-4	133.0	133.6	133.7	134.0	134
C-5	129.3	129.8	130	131.2	131.5
C-6	23.0	23.5	23.7	24.9	24.5
C-7	36.5	37.0	36.2	39.0	-
C-8	83.6	83.7	86.9	86.6	85.0
C-9	37.1	36.9	36.9	38.0	-
C-10	54.1	53.9	54.1	54.6	55.7
C-11	30.2	30.6	30.7	30.8	30.3
C-12	28.2	27	26.8	29.6	27.7
C-13	52.5	51.9	52.1	54.2	50.9
C-14	49.4	48.9	50.1	42.5	49.6
C-15	80.6	80.7	80.8	84.4	81.9
C-16	32.8	-	31.7	33.6	31.6
C-17	18.1	-	18.0	20.9	19.5
C-18	32.1	-	32.1	32.9	32.5
C-19	70.9	67.2	67.1	70.0	-
C-20	20.4	21.4	21.6	22.3	21.9
C-21	151.3	148.8	149.1	150.1	149.9
C-22	168.6	168.8	168.6	167.7	169.8
C-23	65.1	65.5	65.5	66.1	66.6
C-24	29.3	-	28.5	28.4	-
C-36	25.6	-	25.7	26.5	26.6
C-37	32.8	-	33.2	34.1	-
C-38	176	174.5	174.9	177.3	176.8
C-39	42.5	42.6	42.1	42.8	-
C-40	25.3	26.5	27.0	26.5	26.8
C-41	36.5	36.5	36.1	38.2	-
C-42	53.4	50.5	47.6	54.7	54.2
C-43	67.0	70.8	26.1	68.4	68.7
C-44	32.3	32.0	26.4	32.8	-
C-45	37.1	36.0	39.3	38.4	-

Table S2. Stereochemical Diversity Found in Naturally Derived Polycyclic Guanidinium Alkaloids.



compound	type A	type B	type C	type D	origin
ptilomycalin A ¹	X				<i>Crambe crambe</i>
crambescidin 844 ²	X				<i>Crambe crambe</i>
crambescidin 830 ²	X				<i>Crambe crambe</i>
crambescidin 826 ³	X				<i>Monanchora</i> sp.
crambescidin 816 ²	X				<i>Crambe crambe</i>
crambescidin 800 ²	X				<i>Ptilocaulis spiculifer</i> , <i>Hemimycala</i> sp., <i>Batzella</i> sp., <i>Celerina heffernani</i> , <i>Fromia monilis</i>
13,14,15-isocrambescidin 800 ⁴		X			<i>Crambe crambe</i>
crambescidin 431 ⁵	X				<i>Monanchora unguifera</i>
crambescidin 359 ⁵	X				<i>Monanchora unguifera</i>
crambescidic acid/ crambescidin 657 ⁶	X				<i>Monanchora unguifera</i>
13,14,15-isocrambescidin 657 ⁷		X			<i>Crambe crambe</i>
neofolitispace 1 ⁸	X				<i>Neofolitispa dianchora</i>
neofolitispace 2 ⁸	X				<i>Neofolitispa dianchora</i>
neofolitispace 3 ⁸	X				<i>Neofolitispa dianchora</i>
celeromycalin ⁹	X				<i>Celerina heffernani</i>
batzelladine A ¹⁰				X	<i>Batzella</i> sp.
batzelladine B ¹⁰			X		<i>Batzella</i> sp.
batzelladine D ¹⁰				X	<i>Batzella</i> sp.
batzelladine E ¹⁰			X		<i>Batzella</i> sp.
batzelladine F ¹¹				X	<i>Batzella</i> sp.
batzelladine G ¹⁰				X	<i>Batzella</i> sp.
fromiamycalin ⁹	X				<i>Fromia monilis</i>

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