

## Supporting Information for

### Model-free Approach for the Configurational Analysis of Marine Natural Products

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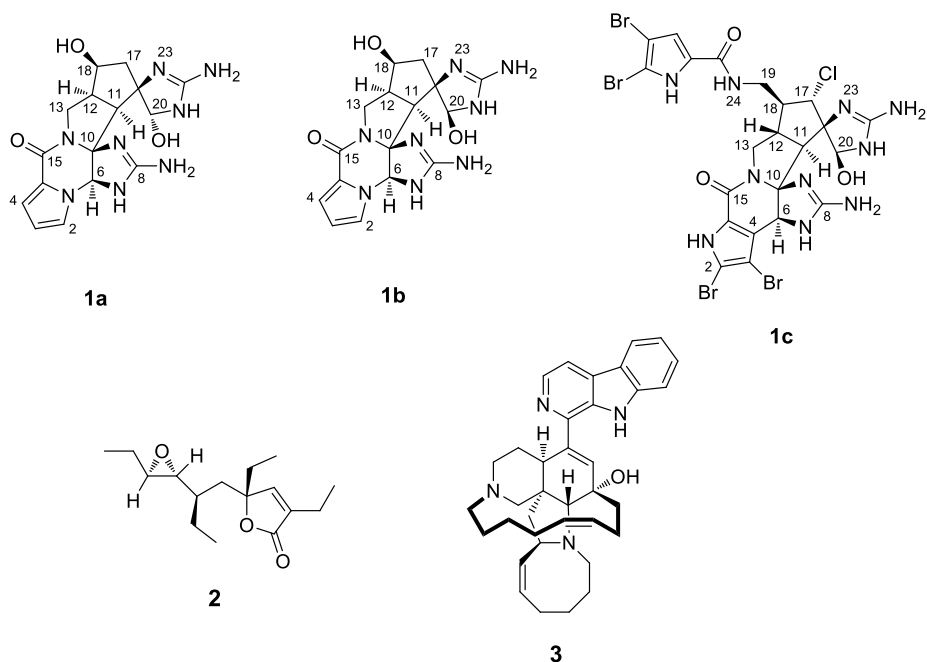
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#### Formulas and Atom Numbering of Compounds 1a-c, 2 and 3



## NOE and Structure Data for Palau'amine Derivatives (1a-c)

The following Tables S1a-c and Figure S1 show the experimental and back-calculated NOE data used for the configurational analysis of the palau'amine derivatives **1a-c**. The Tables were generated directly from the output files for the *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure obtained from configurational and conformational analysis.

Table S1a. NOE data used for **1a**. The experimental data is listed as  $d_{mean}$ , and the allowed lower and upper bonds – here  $d_{mean} \pm 10\%$  – are labeled as  $d_{lower} \dots d_{upper}$ ; the averaged distances back-calculated from *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure data are labelled  $d_{averaged}$ , and the corresponding residuals are listed only if this value falls out of range, i.e.  $d_{averaged} < d_{lower}$  or  $d_{averaged} > d_{upper}$ ; all distance are given in [Å].

	D(averaged)	Deviation	(Percent)	D(lower)	D(mean)	D(upper)	(+/-Range)	Weights	NOE	Contact
NOE [01] =	2.723941	-	( - )	2.36700	2.63000	2.89300	( 10.0%)	1.000000	H5	H6
NOE [02] =	2.616689	-	( - )	2.16900	2.41000	2.65100	( 10.0%)	1.000000	H6	H11
NOE [03] =	2.246777	-	( - )	1.98900	2.21000	2.43100	( 10.0%)	1.000000	H11	H12
NOE [04] =	3.203849	-	( - )	3.01500	3.35000	3.68500	( 10.0%)	1.000000	H11	H13B
NOE [05] =	3.357410	-	( - )	2.76300	3.07000	3.37700	( 10.0%)	1.000000	H11	H17B
NOE [06] =	3.011915	0.041915	( 11.6%)	2.43000	2.70000	2.97000	( 10.0%)	1.000000	H11	H20
NOE [07] =	2.908557	-	( - )	2.57400	2.86000	3.14600	( 10.0%)	1.000000	H12	H13A
NOE [08] =	2.297098	-	( - )	2.03400	2.26000	2.48600	( 10.0%)	1.000000	H12	H13B
NOE [09] =	2.506087	-	( - )	2.50200	2.78000	3.05800	( 10.0%)	1.000000	H12	H17B
NOE [10] =	2.310568	-	( - )	2.24100	2.49000	2.73900	( 10.0%)	1.000000	H12	H18
NOE [11] =	1.766449	-	( - )	1.60200	1.78000	1.95800	( 10.0%)	1.000000	H13A	H13B
NOE [12] =	3.177942	-	( - )	2.81700	3.13000	3.44300	( 10.0%)	1.000000	H13A	H18
NOE [13] =	1.794118	-	( - )	1.60200	1.78000	1.95800	( 10.0%)	1.000000	H17A	H17B
NOE [14] =	2.694828	-	( - )	2.34900	2.61000	2.87100	( 10.0%)	1.000000	H17A	H18
NOE [15] =	2.477978	-	( - )	2.15100	2.39000	2.62900	( 10.0%)	1.000000	H17B	H18
NOE [16] =	2.206491	-0.007509	( -10.3%)	2.21400	2.46000	2.70600	( 10.0%)	1.000000	H17B	H20

Table S1b. NOE data used for **1b**. The experimental data is listed as  $d_{mean}$ , and the allowed lower and upper bonds – here  $d_{mean} \pm 10\%$  – are labeled as  $d_{lower} \dots d_{upper}$ ; the averaged distances back-calculated from *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure data are labelled  $d_{averaged}$ , and the corresponding residuals are listed only if this value falls out of range, i.e.  $d_{averaged} < d_{lower}$  or  $d_{averaged} > d_{upper}$ ; all distance are given in [Å].

	D(averaged)	Deviation	(Percent)	D(lower)	D(mean)	D(upper)	(+/-Range)	Weights	NOE	Contact
NOE [01] =	2.685759	-	( - )	2.35800	2.62000	2.88200	( 10.0%)	1.000000	H5	H6
NOE [02] =	2.428717	0.008717	( 10.4%)	1.98000	2.20000	2.42000	( 10.0%)	1.000000	H6	H11
NOE [03] =	2.396746	-	( - )	2.05200	2.28000	2.50800	( 10.0%)	1.000000	H11	H12
NOE [04] =	2.998957	-0.007043	( -10.2%)	3.00600	3.34000	3.67400	( 10.0%)	1.000000	H11	H13B
NOE [05] =	3.687766	-	( - )	3.09600	3.44000	3.78400	( 10.0%)	1.000000	H11	H17B
NOE [06] =	2.138654	-	( - )	1.87200	2.08000	2.28800	( 10.0%)	1.000000	H11	H20
NOE [07] =	2.820761	-	( - )	2.58300	2.87000	3.15700	( 10.0%)	1.000000	H12	H13A
NOE [08] =	2.358595	-	( - )	2.02500	2.25000	2.47500	( 10.0%)	1.000000	H12	H13B
NOE [09] =	2.614365	-	( - )	2.41200	2.68000	2.94800	( 10.0%)	1.000000	H12	H17B
NOE [10] =	2.326254	-	( - )	2.04300	2.27000	2.49700	( 10.0%)	1.000000	H12	H18
NOE [11] =	3.096064	-	( - )	2.54700	2.83000	3.11300	( 10.0%)	1.000000	H12	H20
NOE [12] =	1.757781	-	( - )	1.60200	1.78000	1.95800	( 10.0%)	1.000000	H13A	H13B
NOE [13] =	3.075460	-	( - )	2.62800	2.92000	3.21200	( 10.0%)	1.000000	H13A	H18
NOE [14] =	1.765112	-	( - )	1.57500	1.75000	1.92500	( 10.0%)	1.000000	H17A	H17B
NOE [15] =	2.740695	-	( - )	2.40300	2.67000	2.93700	( 10.0%)	1.000000	H17A	H18
NOE [16] =	2.410075	-	( - )	2.07900	2.31000	2.54100	( 10.0%)	1.000000	H17B	H18
NOE [17] =	3.214872	0.024872	( 10.9%)	2.61000	2.90000	3.19000	( 10.0%)	1.000000	H17B	H20

Table S1c. NOE data used for **1c**. The experimental data is listed as  $d_{mean}$ , and the allowed lower and upper bonds – here  $d_{mean} \pm 10\%$  – are labeled as  $d_{lower} \dots d_{upper}$ ; the averaged distances back-calculated from *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure data are labelled  $d_{averaged}$ , and the corresponding residuals are listed only if this value falls out of range, i.e.  $d_{averaged} < d_{lower}$  or  $d_{averaged} > d_{upper}$ ; all distance are given in [Å].

	D(averaged)	Deviation	(Percent)	D(lower)	D(mean)	D(upper)	(+/-Range)	Weights	NOE	Contact
NOE [01] =	2.431126	0.011126	( 10.5%)	1.98000	2.20000	2.42000	( 10.0%)	1.000000	H6	H11
NOE [02] =	2.745016	-	( - )	2.25000	2.50000	2.75000	( 10.0%)	1.000000	H11	H13B
NOE [03] =	3.618106	0.021106	( 10.6%)	2.94300	3.27000	3.59700	( 10.0%)	1.000000	H11	H17A
NOE [04] =	2.293836	-	( - )	2.09700	2.33000	2.56300	( 10.0%)	1.000000	H11	H18
NOE [05] =	2.992198	0.011198	( 10.4%)	2.43900	2.71000	2.98100	( 10.0%)	1.000000	H11	H20
NOE [06] =	2.636674	0.007674	( 10.3%)	2.15100	2.39000	2.62900	( 10.0%)	1.000000	H12	H17A
NOE [07] =	2.636882	-	( - )	2.34000	2.60000	2.86000	( 10.0%)	1.000000	H13B	H18
NOE [08] =	3.053332	-	( - )	2.50200	2.78000	3.05800	( 10.0%)	1.000000	H17A	H18
NOE [09] =	3.332277	0.021277	( 10.7%)	2.70900	3.01000	3.31100	( 10.0%)	1.000000	H17A	H20

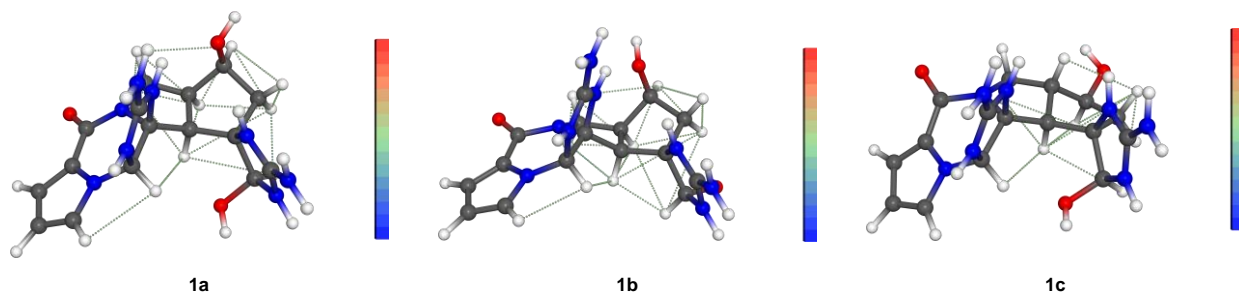


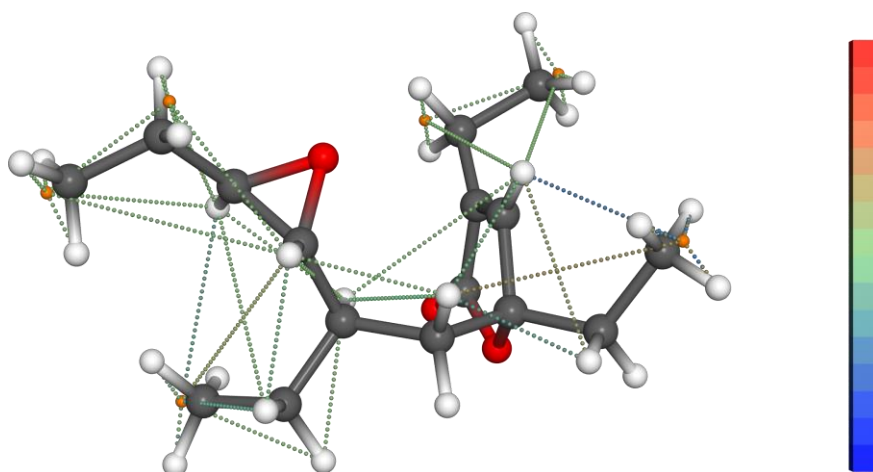
Figure S1. Plot of the best-fit (minimum pseudo energy) DG structures of the palau'amine derivatives **1a-c** with color-coded representation of all NOE contacts used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to +0.40 Å (red).

## NOE and Structure Data for Plakilactone H (2)

The following Table S2 and Figure S2 show the experimental and back-calculated NOE data used for the configurational analysis of the plakilactone (2). The Table was generated directly from the output files for the *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure obtained from configurational and conformational analysis.

Table S2. NOE data used for 2. The experimental data is listed as  $d_{mean}$ , and the allowed lower and upper bounds – here  $d_{mean} \pm 10\%$  – are labeled as  $d_{lower} \cdots d_{upper}$ ; the averaged distances back-calculated from *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure data are labeled  $d_{averaged}$ , and the corresponding residuals are listed only if this value falls out of range, i.e.  $d_{averaged} < d_{lower}$  or  $d_{averaged} > d_{upper}$ ; all distance are given in [Å].

	D(averaged)	Deviation	(Percent)	D(lower)	D(mean)	D(upper)	(+/-Range)	Weights	NOE Contact
NOE [01] =	2.644129	-	( - )	2.47500	2.75000	3.02500	( 10.0%)	1.000000	H16A H16B H16C    H15B
NOE [02] =	2.913799	-0.074201	( -12.2%)	2.98800	3.32000	3.65200	( 10.0%)	1.000000	H16A H16B H16C    H8
NOE [03] =	3.465938	0.011938	( 10.4%)	2.82600	3.14000	3.45400	( 10.0%)	1.000000	H3    H11A H11B
NOE [04] =	2.588254	-0.021746	( -10.7%)	2.61000	2.90000	3.19000	( 10.0%)	1.000000	H3    H5B
NOE [05] =	3.209843	0.074843	( 12.6%)	2.56500	2.85000	3.13500	( 10.0%)	1.000000	H3    H13A
NOE [06] =	3.529531	0.009531	( 10.3%)	2.88000	3.20000	3.52000	( 10.0%)	1.000000	H3    H12A H12B H12C
NOE [07] =	2.647202	-0.151798	( -14.9%)	2.79900	3.11000	3.42100	( 10.0%)	1.000000	H3    H14A H14B H14C
NOE [08] =	3.565704	0.023704	( 10.7%)	2.89800	3.22000	3.54200	( 10.0%)	1.000000	H3    H6
NOE [09] =	2.845071	-	( - )	2.41200	2.68000	2.94800	( 10.0%)	1.000000	H8    H9A H9B
NOE [10] =	2.955072	-	( - )	2.88900	3.21000	3.53100	( 10.0%)	1.000000	H8    H10A H10B H10C
NOE [11] =	2.470103	-	( - )	2.08800	2.32000	2.55200	( 10.0%)	1.000000	H8    H6
NOE [12] =	2.481681	-	( - )	2.37600	2.64000	2.90400	( 10.0%)	1.000000	H7    H5B
NOE [13] =	2.649766	-	( - )	2.38500	2.65000	2.91500	( 10.0%)	1.000000	H7    H9A H9B
NOE [14] =	2.441980	-0.015020	( -10.6%)	2.45700	2.73000	3.00300	( 10.0%)	1.000000	H7    H15A
NOE [15] =	3.840827	-	( - )	3.18600	3.54000	3.89400	( 10.0%)	1.000000	H7    H10A H10B H10C
NOE [16] =	3.874147	0.090147	( 12.6%)	3.09600	3.44000	3.78400	( 10.0%)	1.000000	H7    H16A H16B H16C
NOE [17] =	3.102404	-	( - )	2.64600	2.94000	3.23400	( 10.0%)	1.000000	H7    H6
NOE [18] =	2.352820	-0.050180	( -11.9%)	2.40300	2.67000	2.93700	( 10.0%)	1.000000	H5B    H13A
NOE [19] =	2.903985	-0.003015	( -10.1%)	2.90700	3.23000	3.55300	( 10.0%)	1.000000	H5B    H6
NOE [20] =	3.489705	0.145705	( 14.8%)	2.73600	3.04000	3.34400	( 10.0%)	1.000000	H5B    H14A H14B H14C
NOE [21] =	2.676060	-	( - )	2.67300	2.97000	3.26700	( 10.0%)	1.000000	H15B    H8
NOE [22] =	3.807998	0.023998	( 10.7%)	3.09600	3.44000	3.78400	( 10.0%)	1.000000	H15A    H8
NOE [23] =	2.632971	-	( - )	2.46600	2.74000	3.01400	( 10.0%)	1.000000	H9A H9B    H10A H10B H10C
NOE [24] =	2.621216	-0.096784	( -13.2%)	2.71800	3.02000	3.32200	( 10.0%)	1.000000	H15A    H16A H16B H16C
NOE [25] =	2.616184	-	( - )	2.48400	2.76000	3.03600	( 10.0%)	1.000000	H12A H12B H12C    H11A H11B



2

Figure S2. Plot of the best-fit (minimum pseudo energy) DG structures of plakilactone H (2) with color-coded representation of all NOE contacts used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to +0.40 Å (red).

## NOE and Structure Data for Manzamine A (3)

The following Table S3-4 and Figure S3 show the experimental and back-calculated NOE and RDC data used for the configurational analysis of the manzamine A (**3**). The Table was generated directly from the output files for the *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure obtained from configurational and conformational analysis.

Table S3. NOE data used for **3**. The experimental data is listed as  $d_{mean}$ , and the allowed lower and upper bounds – here  $d_{mean} \pm 10\%$  – are labeled as  $d_{lower}$  ...  $d_{upper}$ ; the averaged distances back-calculated from *ConArch*<sup>+</sup>/*DG* best-fit (minimum pseudo energy) structure data are labeled  $d_{averaged}$ , and the corresponding residuals are listed only if this value falls out of range, i.e.  $d_{averaged} < d_{lower}$  or  $d_{averaged} > d_{upper}$ ; all distance are given in [Å].

NOE	D(averaged)	Deviation	(Percent)	D(lower)	D(mean)	D(upper)	(+/-Range)	Weights	NOE Contact
NOE[01]	2.476617	-	( - )	2.02700	2.25200	2.47700	( 10.0%)	1.000000	H14A H14B    H26
NOE[02]	2.797847	-	( - )	2.61400	2.90400	3.19400	( 10.0%)	1.000000	H17A H17B    H26
NOE[03]	2.497658	-	( - )	2.29800	2.55300	2.80800	( 10.0%)	1.000000	H26    H28A H28B
NOE[04]	2.570980	-	( - )	2.30500	2.56100	2.81700	( 10.0%)	1.000000	H26    H36A H36B
NOE[05]	2.159208	-	( - )	1.93200	2.14700	2.36200	( 10.0%)	1.000000	H30A H30B    H34
NOE[06]	2.226290	-	( - )	1.99800	2.22000	2.44200	( 10.0%)	1.000000	H32    H33
NOE[07]	2.742605	-	( - )	2.40400	2.67100	2.93800	( 10.0%)	1.000000	H33    H35A H35B
NOE[08]	2.449948	-	( - )	2.02600	2.25100	2.47600	( 10.0%)	1.000000	H33    H36A H36B
NOE[09]	2.558147	-	( - )	2.28000	2.53300	2.78600	( 10.0%)	1.000000	H34    H35A H35B

Table S4. RDC data used for **3**. The experimental data is listed as  $D_{exp}$ , and the RDCs back-calculated from the structure model are labeled  $D_{calc}$ . All values including the Monte-Carlo derived error esitiomates are given in [Hz].

Results for Multi-Parameter SVD Fit of Calculated and Experimental Data:				D(exp)-D(calc)		Normalized Weights		Atom Labels	
D[01]	d(calc) [Hz]	+/- Error	D(exp) [Hz]	+/- Error	Rel. Weights	r[01]	w[01]		
D[01]	21.704870	1.245029	21.823309	0.500000	1.000000	r[01]	w[01]	C3-H3	
D[02]	0.137062	1.671443	0.091663	0.500000	1.000000	r[02]	w[02]	C4-H4	
D[03]	21.655839	1.096703	21.786998	0.500000	1.000000	r[03]	w[03]	C5-H5	
D[04]	-26.334976	1.461292	-26.566153	0.500000	1.000000	r[04]	w[04]	C6-H6	
D[05]	-6.583622	1.763345	-6.649118	0.500000	1.000000	r[05]	w[05]	C7-H7	
D[06]	-22.529338	1.052731	-22.695334	0.500000	1.000000	r[06]	w[06]	C8-H8	
D[07]	1.945254	1.370447	1.886530	0.500000	1.000000	r[07]	w[07]	C11-H11	
D[08]	22.670474	1.481094	22.847812	0.500000	1.000000	r[08]	w[08]	C13-H13A+C13-H13B	
D[09]	23.926041	1.398360	24.107193	0.500000	1.000000	r[09]	w[09]	C14-H14A+C14-H14B	
D[10]	9.241049	1.107958	9.331405	0.500000	1.000000	r[10]	w[10]	C15-H15	
D[11]	-27.621917	1.440511	-27.669637	0.500000	1.000000	r[11]	w[11]	C16-H16	
D[12]	-39.585065	1.967031	-39.747489	0.500000	1.000000	r[12]	w[12]	C17-H17A+C17-H17B	
D[13]	-40.930775	1.964931	-41.123129	0.500000	1.000000	r[13]	w[13]	C18-H18A+C18-H18B	
D[14]	12.472912	1.653159	12.535599	0.500000	1.000000	r[14]	w[14]	C19-H19A+C19-H19B	
D[15]	40.418646	1.296505	40.598288	0.500000	1.000000	r[15]	w[15]	C20-H20A+C20-H20B	
D[16]	-9.743054	1.726061	-9.846516	0.500000	1.000000	r[16]	w[16]	C22-H22A+C22-H22B	
D[17]	27.387241	1.667193	27.491775	0.500000	1.000000	r[17]	w[17]	C23-H23A+C23-H23B	
D[18]	-8.335456	1.500358	-8.231811	0.500000	1.000000	r[18]	w[18]	C24-H24	
D[19]	-30.251677	1.408419	-30.525030	0.500000	1.000000	r[19]	w[19]	C26-H26	
D[20]	-6.911463	1.824540	-6.919452	0.500000	1.000000	r[20]	w[20]	C28-H28A+C28-H28B	
D[21]	5.251709	1.918694	5.197804	0.500000	1.000000	r[21]	w[21]	C29-H29A+C29-H29B	
D[22]	9.627178	2.190704	9.674817	0.500000	1.000000	r[22]	w[22]	C30-H30A+C30-H30B	
D[23]	-22.660937	2.127970	-22.765273	0.500000	1.000000	r[23]	w[23]	C31-H31A+C31-H31B	
D[24]	2.729423	1.233013	2.762687	0.500000	1.000000	r[24]	w[24]	C32-H32	
D[25]	8.710639	1.522551	8.639642	0.500000	1.000000	r[25]	w[25]	C33-H33	
D[26]	-28.729280	1.548104	-28.870231	0.500000	1.000000	r[26]	w[26]	C34-H34	
D[27]	4.847359	1.544533	4.742710	0.500000	1.000000	r[27]	w[27]	C35-H35A+C35-H35B	
D[28]	33.787954	1.525093	33.909669	0.500000	1.000000	r[28]	w[28]	C36-H36A+C36-H36B	

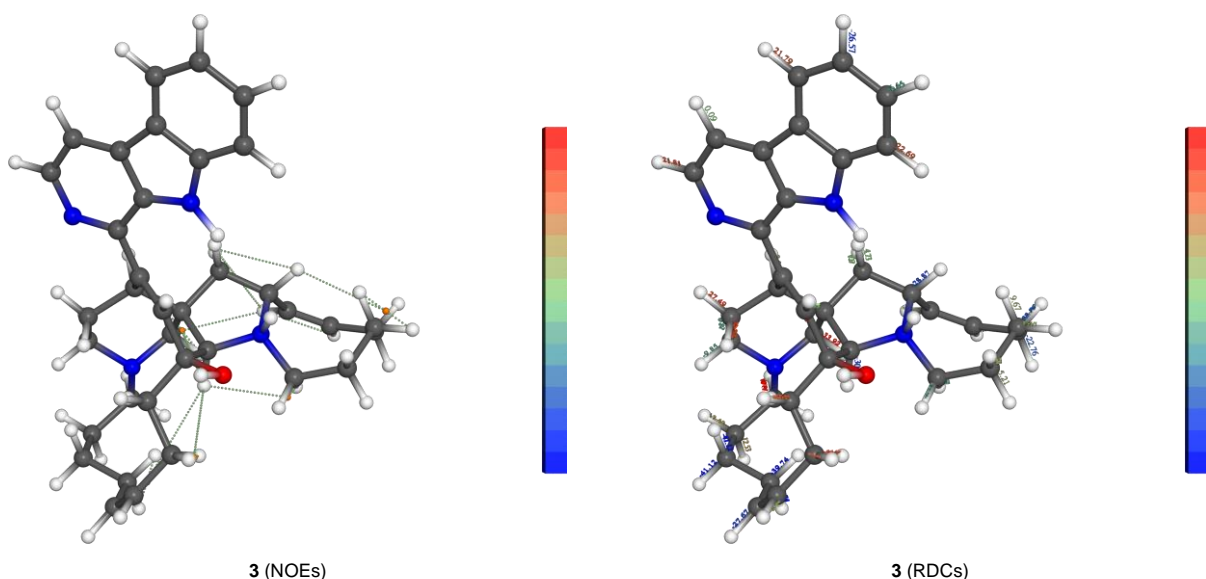
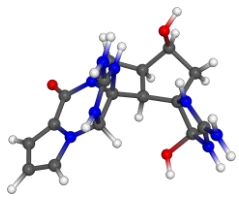
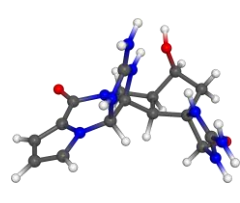
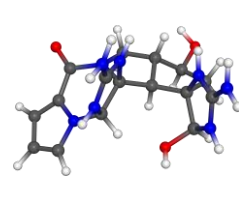
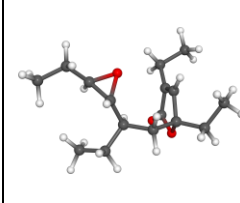
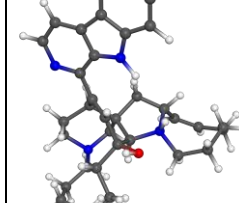


Figure S3. Plot of the best-fit (minimum pseudo energy) *DG* structures of manzamine A (**3**) with color-coded representation of all NOE contacts (left model) and all RDCs (right model) used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to +0.40 Å (red), or to the range of RDCs (blue: -40 Hz, red: +40 Hz) back-calculated for **3**.

# Atomic Coordinates for Compounds 1a-c, 2 and 3

The following tables provide the atomic coordinates for the final best-fit (minimum pseudo energy) DG structures of **1a-c**, **2**, and **3**, copy-and-paste for further usage:

Table S5. rDG best-fit structures (atomic coordinates) for compounds **1a-c**, **2**, and **3**.

Palau'amine Derivatives				Plakilactone H			Manzamine A		
1a	1b	1c		2		3			
									
N1 -0.933681 2.737943 -0.294880 C2 -2.327504 2.652587 -0.295406 C3 -1.840589 3.937060 -0.124628 C4 -1.726753 4.828516 -0.017523 C5 -0.567493 4.077740 -0.123622 C6 -0.090870 1.651889 -0.444655 N7 0.789913 1.793511 -1.693290 C8 0.688092 0.616321 -2.459749 N9 -0.133854 -0.278790 -1.857730 C10 -0.698665 0.231364 -0.543149 C11 -0.518545 -0.776389 0.624302 C12 -1.612086 -1.794176 0.465759 C13 -2.736412 -1.118413 -0.297383 N14 -2.164012 0.239200 -0.625665 C15 -3.011129 1.367291 -0.457015 O15 -4.226925 1.218094 -0.454890 C16 0.777670 -1.498804 1.095579 C17 0.308559 -1.048964 1.092420 C18 -0.892333 -3.107023 0.063254 O19 -0.330984 -1.093276 -1.235419 C20 1.270668 -1.097048 2.537806 O20 0.614343 0.165685 2.918561 N21 2.690393 -0.870742 2.350390 C22 3.068106 -1.094145 1.032250 H22 4.320063 -0.818670 0.617529 N23 2.014157 -1.342081 0.296894 H23 -3.901094 4.185663 -0.084505 H4 -1.771515 5.908476 0.123135 H5 0.480699 4.375113 -0.092890 H6 0.679798 1.700390 0.382579 H7 1.332023 2.538880 -1.938675 H8 -0.354584 -1.137093 -2.110970 H11 -0.770016 -0.171385 1.459824 H12 -2.063670 -2.049165 2.449707 H18 -1.533084 -3.968626 0.250814 H19X -0.207042 -3.997763 -1.581631 H20 0.987717 -1.815280 3.307339 H20X 1.319692 0.748939 3.216970 H21 3.334601 -0.589670 3.077442 H23 2.073005 -1.521495 -0.684335 H24 1.930731 1.154593 -3.994877 H28 1.219313 -0.423623 -4.138617 H34 -1.028787 -1.590808 -1.231784 H38 -3.638027 -0.929405 0.285255 H7A 1.108561 -3.672912 0.659941 H7B 0.020103 -3.380588 2.098883 H2A 3.070192 -0.361122 1.258067 H2B 4.563686 -0.927383 -0.364095	N1 2.091626 -2.095249 -0.009804 C2 1.399632 -3.308700 0.053678 C3 2.737644 -4.328880 -0.292816 C4 3.544757 -3.722375 -0.575477 C5 3.411441 -2.355007 -0.397425 C6 1.527447 -0.811682 0.268337 N7 2.057408 -0.214513 1.538476 C8 1.056191 0.123108 2.317653 N9 1.745803 0.674015 3.584357 N9 -0.140149 -0.170085 1.832234 C10 -0.020141 -0.778115 0.457233 C11 -0.983589 -0.004952 -0.624244 C12 -2.736409 -1.794176 0.465759 C13 -2.061338 -2.032744 -0.157276 N14 -0.669448 -2.070668 0.406129 C15 -0.015474 -3.350665 0.434225 O15 -0.639248 -4.336910 0.753742 C16 0.995040 1.531685 -0.821584 C17 -2.476491 1.808959 -0.275905 C18 -2.972564 0.485762 0.396232 O19 -2.949095 0.488727 1.744935 C20 -0.868880 2.025538 -2.316658 O20 -2.112162 2.650406 -2.743613 N21 0.203078 3.010494 -2.262097 C22 0.656161 2.205368 -0.999688 H22 1.624155 4.074233 -0.680134 N23 0.001144 -2.411396 -0.142307 H23 0.064500 -5.388257 -0.334347 H4 4.466244 -4.237225 -0.879216 H5 4.133522 -1.546879 -0.511653 H6 1.830139 -0.166320 -0.566676 H7 3.040836 -0.085725 1.748604 H9 -0.986914 -0.006841 2.257314 H11 -0.382005 -0.334824 -1.554953 H12 -2.722041 -0.481047 -1.451320 H18 -0.105102 0.359608 0.300540 H19X 3.717340 1.202390 -3.009081 H20 -0.692370 1.949300 -3.049317 H20X -2.712366 3.949300 -3.049317 H21 0.494910 3.527944 -3.057124 H23 0.192817 2.376127 0.817675 H24 2.182720 0.870187 3.936546 H28 0.462819 0.913316 4.185017 H34 -2.738404 -2.404187 0.611932 H38 -2.132644 -2.708002 -1.009944 H7A 2.501009 2.614405 0.458094 H7B -3.127523 2.085798 -1.105132 H2A 2.077139 4.646041 -2.391451 H2B 1.938862 4.192162 0.280521	N1 -1.127977 -2.573854 0.934884 C2 -0.273816 3.554316 0.406062 C3 -0.458757 -4.723708 1.121387 C4 -1.456440 -4.463778 2.119301 C5 -1.850509 -3.143847 1.988028 C6 -1.239844 -1.239054 0.480210 N7 -2.447648 -0.974252 -0.340560 C8 -2.147452 -0.457724 -1.536808 N9 -3.070133 -0.142752 -2.471943 N9 -0.824863 -0.311977 -1.696237 C10 -0.049560 -0.754856 -0.467513 C11 0.896581 0.235511 0.076153 C12 2.116544 0.119138 -0.646418 C13 2.320984 -1.810755 -0.817553 N14 0.878801 -1.810755 -0.817553 C15 0.611939 3.228758 -0.217870 O15 1.101660 -3.997646 -1.497506 C16 0.978986 1.889136 0.692721 C17 2.545468 2.624499 0.422314 C18 3.191248 0.394414 0.256298 O19 4.410537 1.88201 0.385996 C20 0.005362 2.324988 1.560320 O20 -0.657141 1.214069 2.165883 N21 -0.932422 3.181665 1.051944 C22 0.828296 3.484086 -0.286492 N22 -1.578716 4.327661 -1.006640 N23 0.141895 2.680085 -0.778374 H3 0.064500 -5.66371 0.946140 H4 -1.836780 -5.174476 2.853024 H5 -2.581801 -2.556796 2.547182 H6 -1.254990 -0.604647 1.366437 H7 -3.392020 -1.170922 -0.033366 H9 -0.38710 0.043431 -2.472547 H11 1.070511 0.025957 1.107564 H12 2.245751 0.629052 -1.627908 H18 3.335734 0.425540 1.198379 H19X 4.662123 0.615304 -1.048950 H20 0.686957 2.763887 2.308461 H20X -1.549857 1.485340 2.467483 H21 1.606439 3.813200 1.622028 H23 0.382644 2.664742 -1.748565 H24 -0.065035 -0.281281 -2.294501 H28 -2.808183 0.243891 -3.747688 H34 2.864721 -1.746198 -1.697978 H38 2.751156 1.881391 0.606774 H7A 2.623272 2.929792 -0.596599 H7B 2.541822 2.765464 1.371030 H2A -2.96136 4.900203 -0.570071 H2B -1.462742 4.41316 2.014490	C1 1.424495 0.714735 2.153258 C2 2.078856 0.667628 0.775509 C3 1.378837 1.423829 -0.027627 C4 0.176689 2.065965 0.738694 C5 -1.147998 1.410698 0.208326 C6 -1.282218 -0.124005 0.588028 C7 -1.227633 -0.790652 -0.101587 C8 -0.656363 -2.191297 -1.167335 C9 -1.113856 -3.094760 -2.327058 C10 -2.081511 -4.020237 -1.831242 C11 3.327075 -0.162759 0.564266 C12 4.592323 0.715244 0.245659 C13 0.115803 3.375032 0.498000 C14 1.132855 4.169717 -0.601417 C15 -2.632986 -0.537826 1.081117 C16 2.681570 -1.948428 1.641498 O1 0.443413 1.741198 2.076345 O2 1.642172 0.078907 3.125915 O3 0.093860 -1.012633 -1.544003 H5 1.411739 1.742716 -1.069148 H5A -1.998891 1.946106 0.629529 H5B -1.165259 1.620959 -0.861064 H6 -0.447534 -0.525177 0.958885 H7 -2.033227 -0.544407 -1.707596 H8 -0.399640 -2.688698 -0.230325 H8A -0.228583 -3.539513 -2.781577 H8B -1.602633 -2.463607 -3.068940 H10A -2.752945 -3.815329 -1.063996 H10B -2.680644 -4.576428 -2.655629 H10C -1.532335 -5.040990 -1.405740 H11A 3.176275 -0.801371 -0.306098 H11B 3.479779 -0.805265 1.430684 H12A 4.349198 1.585637 -0.283769 H12B 5.002486 1.059731 1.274927 H12C 5.358387 0.136782 -0.190703 H13A -0.818118 3.762910 0.048457 H13B 0.273368 4.130857 1.425672 H14A 2.203332 4.235340 -0.473495 H14B 0.657511 3.945617 -1.360809 H14C 0.770014 5.201028 -0.601228 H15B -2.857561 0.214199 1.856878 H3 0.105762 -0.094742 -1.895267 H3A -1.388959 2.203546 -2.885574 H4 -0.561417 4.645963 -0.037079 H5 -3.159049 7.161556 -2.827942 H5A -1.578409 8.968854 -2.344228 H5B 0.489707 8.528372 -1.056628 H8 1.011548 6.232973 -0.202652 H9 0.034589 3.547823 -0.108228 H11 -1.094913 2.184836 2.067227 H12 -0.034294 1.384420 2.893263 H13A -1.864938 -1.382479 1.727440 H13B -1.864285 -0.205091 2.756605 H14 0.028597 -0.577670 4.234647 H15 -1.537874 -2.101541 5.249140 H16 -2.010108 -4.232782 4.397399 H17A -0.188250 -3.665756 2.083941 H17B -0.344933 -5.257237 2.862798 H18A -2.715092 -5.369475 2.233919 H18B -2.574341 -3.746202 1.453448 H19A -1.219963 -6.335742 0.595802 H19B -2.548318 -5.478295 -0.235504 H20A 0.368423 -4.744591 -0.078016 H20B -0.685024 -4.926001 -1.502796 H21 3.006769 -3.988080 -0.522320 H22B -2.324785 -2.980004 -2.088454 H23A -2.674753 -1.207815 0.368339 H23B -3.448720 -0.012174 -2.242763 H24 -1.565399 -0.254921 -2.242763 H25 0.813734 -6.525887 0.968368 H27 2.072956 1.058895 0.482505 H28A 2.652552 -0.692505 2.169309 H28B 3.442090 -1.518989 0.785526 H29A 4.056084 1.311923 1.711111 H29B 5.010167 -0.174308 0.062924 H30A 4.617540 1.258988 -0.592800 H30B 6.109852 1.077135 0.360624 H31A 6.162899 -1.253077 -0.106400 H31B 6.274387 -0.243471 -1.560033 H32 4.078006 -2.361224 -1.863683 H33 2.801564 -2.097816 -2.235719 H34 3.046039 0.376942 -1.895397 H35A 0.640548 0.926076 -1.967680 H35B 1.012910 -0.517675 -2.899867 H36A 1.064391 -2.840967 -1.007347 H36B -0.076012 -2.575719 -2.347520						