Supporting Information for

The advanced floating chirality distance geometry approach – how anisotropic NMR parameters can support the determination of the relative configuration of natural products

Matthias Köck[a], Michael Reggelin[b], and Stefan Immel[b]

[a] Alfred-Wegener-Institut für Polar- und Meeresforschung in der Helmholtz-Gemeinschaft, Am Handelshafen 12, 27570 Bremerhaven, Germany

[b] Clemens-Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Alarich-Weiss-Straße 4, 64287 Darmstadt, Germany

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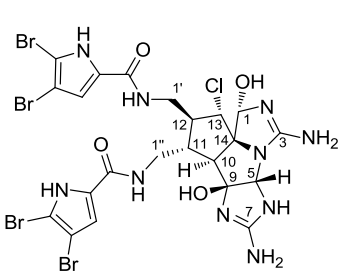
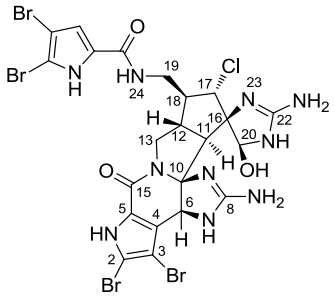
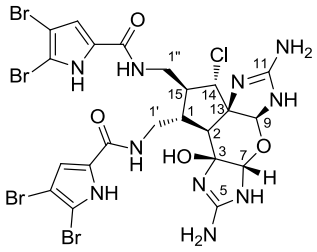
Formulas and Atom Numbering of Compounds (1)-(5)



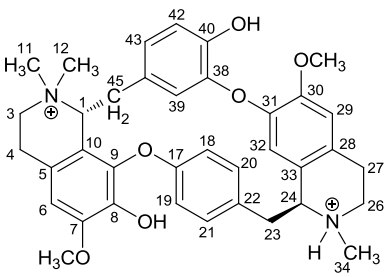
Axinellamine A (**1**)



Tetrabromostyloguanidine (**2**)



3,7-*epi*-Massadine chloride (**3**)



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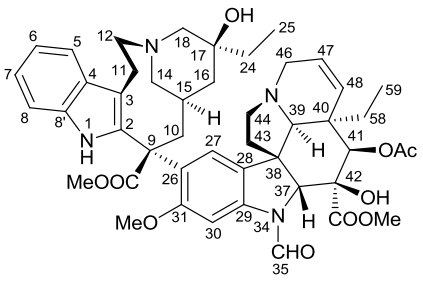
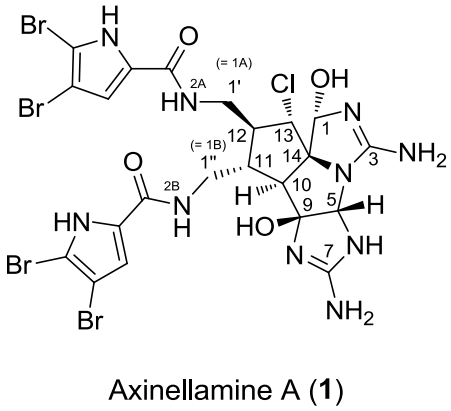


Vincristine (**5**)

NOE and Structure Data for Axinellamine A (1)

Table S1. NOE data used for Axinellamine (**1**) ($N = 37$ NOEs, the NMR-derived expectation values are denoted as d_{mean}, and the allowed lower and upper bonds – usually $d_{mean} \pm 10\%$ – are labeled as $d_{min} \cdots d_{max}$; the averaged distances back-calculated from structural data are labelled d_{calc}, and the corresponding residuals are listed only if this value falls out of range, i.e. $d_{calc} < d_{min}$ or $d_{calc} > d_{max}$; all distance are given in [Å]). The NOE labels refer to the formula shown on the right, where given as e.g. $H^A|H^B$, NOEs were recalculated from structures as r^{-6} averages over all pairs of atom-atom distances.

NOE		distances [Å]			
		d_{mean}	$d_{min} \cdots d_{max}$	d_{calc}	Δd
H1	H10	3.319	2.987-3.651	3.662	0.011
H1	H12	2.499	2.249-2.749	2.617	-
H2	H1	2.655	2.390-2.921	2.475	-
H2	H1X	3.577	3.219-3.935	3.673	-
H5	H11	3.859	3.473-4.245	4.314	0.069
H5	H13	2.768	2.491-3.044	2.472	-0.019
H5	H31	3.795	3.415-4.174	4.210	0.036
H6	H5	2.609	2.348-2.870	2.504	-
H6	H71	3.091	2.782-3.400	2.741	-0.041
H8	H10	2.837	2.554-3.121	2.651	-
H8	H11	4.014	3.612-4.415	3.681	-
H8	H71	3.300	2.970-3.630	3.644	0.014
H8	H9X	3.494	3.144-3.843	3.215	-
H10	H12	3.562	3.206-3.919	3.682	-
H10	H5	3.651	3.286-4.016	3.844	-
H13	H10	3.526	3.173-3.878	3.738	-
H13	H11	2.678	2.410-2.945	3.089	0.144
H13	H1A1	2.593	2.334-2.852	2.934	0.082
H1X	H1	2.316	2.084-2.547	2.388	-
H1X	H10	2.567	2.310-2.824	2.332	-
H9X	H10	4.149	3.734-4.564	3.888	-
H9X	H11	3.083	2.775-3.391	3.402	0.011
H9X	H13	3.373	3.036-3.711	3.048	-
H9X	H5	2.432	2.189-2.675	2.208	-
H32	H5	3.364	3.028-3.700	2.995	-0.033
H1A1	H12	2.825	2.542-3.107	2.597	-
H1A2	H11	2.648	2.383-2.913	2.760	-
H1A2	H12	2.534	2.280-2.787	2.369	-
H1A2	H1A1	1.780	1.602-1.958	1.850	-
H2A	H11	3.042	2.737-3.346	3.096	-
H2A	H12	3.660	3.294-4.026	4.002	-
H2A	H13	2.716	2.445-2.988	2.438	-0.007
H2A	H1A1	2.625	2.362-2.887	2.429	-
H2B	H10	3.148	2.833-3.463	3.798	0.335
H2B	H11	2.770	2.493-3.047	2.261	-0.232
H2B	H12	3.328	2.995-3.660	3.791	0.131
H2B	H1A2	2.804	2.524-3.085	3.189	0.104



Axinellamine A (**1**)

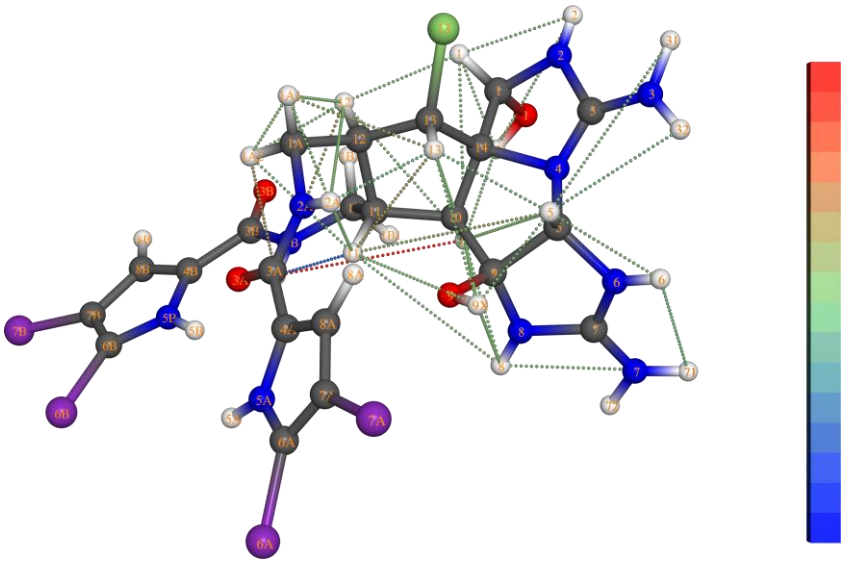


Figure S1. Plot of the best-fit (minimum pseudo energy) DG structure of Axinellamine A (**1**) with color-coded representation of all NOE contacts used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to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

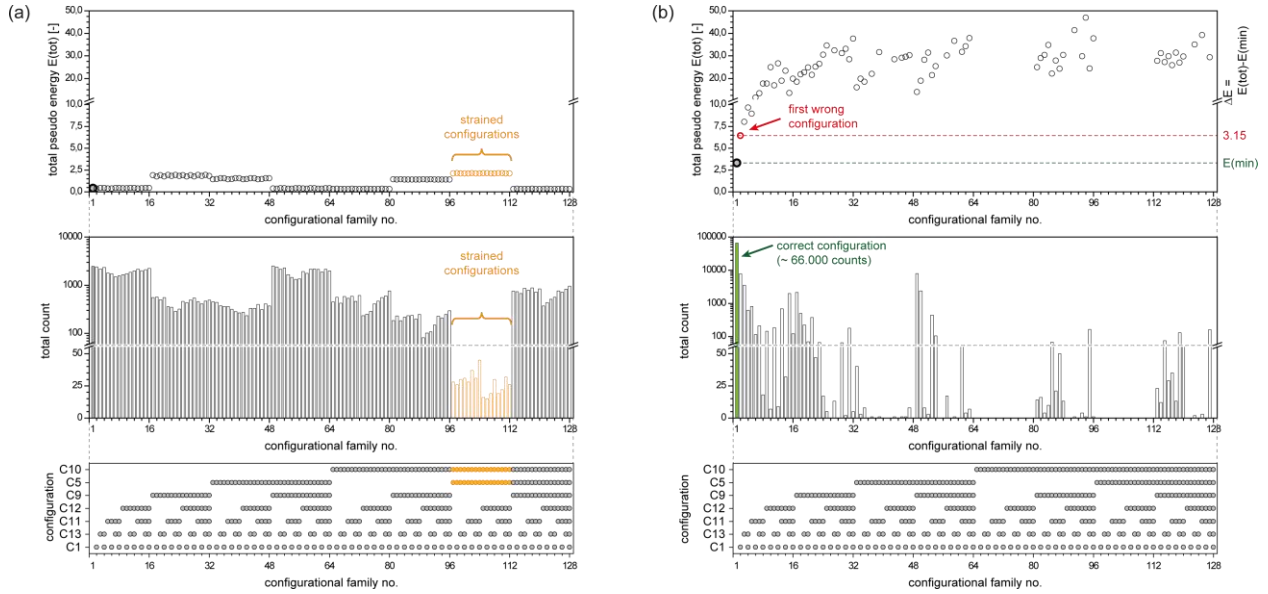


Figure S2.

(a) For Axinellamine A (**1**), an extended unrestricted floating-chirality DG calculation (100.000 structures) produces all 128 diastereomers (eight stereogenic centers, 2^{N-1} configurational families, only C14 was fixed in its configuration in order to avoid enantiomeric structures). In this simulation, only holonomic distance bounds (bond lengths) were used as restraints, and no NOE information was used to restrict configurational (and conformational) space. The *top plot* shows the minimum holonomic pseudo energy of each of the 128 diastereomers, and the *center plot* provides an overview on the total number (counts as columns) of structures generated in this simulation for each configuration. The *bottom plot* identifies each configuration generated: The rows of filled circles indicate for each configurational family which stereogenic center (C1, C13, C11, C12, C9, C5, and C10) is inverted in relation to the correct configuration of Axinellamine A (**1**, the correct configuration is labeled no. #1 on the left side of the plots), a missing circle indicates retention of stereogenic centers as compared to **1**. The DG approach samples even highly strained configurations (marked in orange, configurations no. #97-112), albeit these occur with significantly lower statistical sampling rates. In all these 16 highly strained diastereomers, at least C5 and C10 feature an inverted configuration, which leads to a two-fold *trans*-anellation of two of the five-membered rings (see Figure S3 below for a superposition plot of these structures).

(b) Using NOE data for Axinellamine (**1**) ($N = 37$ NOEs), an extended floating-chirality DG calculations (100.000 structures) produced 74 out of the 128 possible diastereomers, the *center* and *bottom plot* and visualize the individual configurational families and their relative counts as described in (a). The left most column displays the sampling rate for the correct configuration of Axinellamine A (**1**, about 66.000 correct structures were generated in this rDG simulation, note the logarithmic scale after the axis break), whereas the sampling rate of wrong configurations significantly drops as the total pseudo energy raises. The *top plot* shows the minimum total error (= pseudo energy) for each configurational family, the correct structure (left most entry labeled no. #1, large black circle) emerges as the global pseudo energy minimum structure ($E_{min} = 3.30$), the first wrong configuration (wrong configuration at C1, red circle) features a significantly higher pseudo energy ($\Delta E = 3.15$), and any alternate diastereomer is characterized by even higher pseudo energies (note the break in the scale of the axis). Nevertheless, DG efficiently samples all possible configurations under the restraints of the experimental NOE data, and the correct configuration of **1** emerges as the best-fit, lowest pseudo energy structure from all rDG simulations described here.

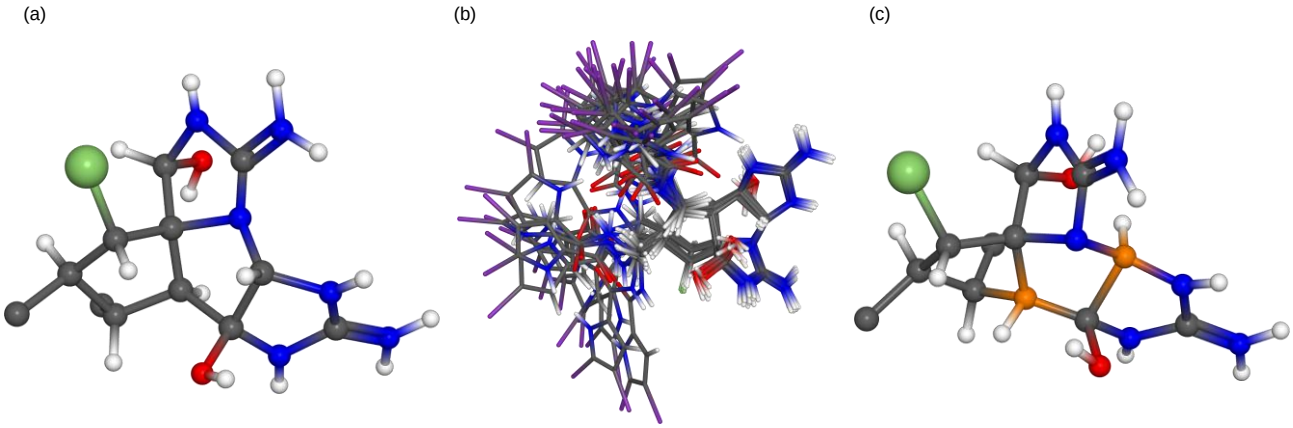
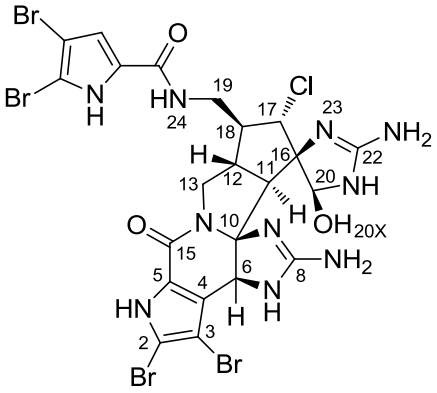


Figure S3. (a) Plot of central ring structure of Axinellamine A (**1**) with correct configuration of all stereogenic centers as identified from the rDG simulation described in Figure S2b; this structure is identical to the one shown in Figure S1. (b) Superposition of 16 highly strained diastereomers of **1**, identified from the unrestricted DG simulation as described in Figure S2a, and marked in these plots in orange. All these highly distorted structures feature a wrong configuration at C5 and C10 (atoms marked in orange in the plot on the right side (c)), and the structure shown in (c) corresponds to the configurational family labeled no. #97 in Figure S2b.

NOE and Structure Data for Tetrabromostyloguanidine (2)

Table S2. NOE data used for Tetrabromostyloguanidine (**2**) ($N = 27$ NOEs, the NMR-derived expectation values are denoted as d_{mean}, and the allowed lower and upper bonds – usually $d_{mean} \pm 10\%$ – are labeled as $d_{min} \cdots d_{max}$; the averaged distances back-calculated from structural data are labelled d_{calc}, and the corresponding residuals are listed only if this value falls out of range, i.e. $d_{calc} < d_{min}$ or $d_{calc} > d_{max}$; all distance are given in [Å]). The NOE labels refer to the formula shown on the right, where given as e.g. $H^A|H^B$, NOEs were recalculated from structures as r^{-6} averages over all pairs of atom-atom distances.

NOE		distances [Å]			
		d_{mean}	$d_{min} \cdots d_{max}$	d_{calc}	Δd
H6	H20X	2.720	2.450-2.990	2.720	-
H6	H7	2.460	2.210-2.710	2.385	-
H6	H9	4.030	3.630-4.430	4.024	-
H11	H132	2.500	2.250-2.750	2.766	0.016
H11	H17	3.270	2.940-3.600	3.625	0.025
H11	H20X	2.935	2.650-3.220	2.674	-
H11	H6	2.200	1.980-2.420	2.592	0.172
H11	H9	3.580	3.220-3.940	3.925	-
H12	H9	2.360	2.120-2.600	2.395	-
H17	H12	2.390	2.150-2.630	2.442	-
H17	H191	2.840	2.560-3.120	3.338	0.218
H17	H192	2.400	2.100-2.700	2.051	-0.049
H17	H20	3.010	2.710-3.310	3.492	0.182
H17	H23	2.320	2.090-2.550	2.612	0.062
H17	H24	3.050	2.750-3.350	3.393	0.043
H18	H11	2.330	2.100-2.560	2.415	-
H18	H132	2.600	2.340-2.860	2.600	-
H18	H17	2.780	2.500-3.060	3.035	-
H18	H20	3.110	2.800-3.420	3.427	0.007
H18	H23	4.350	3.910-4.790	4.743	-
H18	H24	2.950	2.650-3.250	2.894	-
H20	H11	2.710	2.440-2.980	3.008	0.028
H20	H20X	2.180	1.990-2.370	2.338	-
H20	H21	2.530	2.280-2.780	2.470	-
H23	H6	4.300	3.870-4.730	4.474	-
H23	H9	3.220	2.900-3.540	2.877	-0.023
H27	H24	2.340	2.110-2.570	2.191	-



Tetrabromostyloguanidine (**2**)

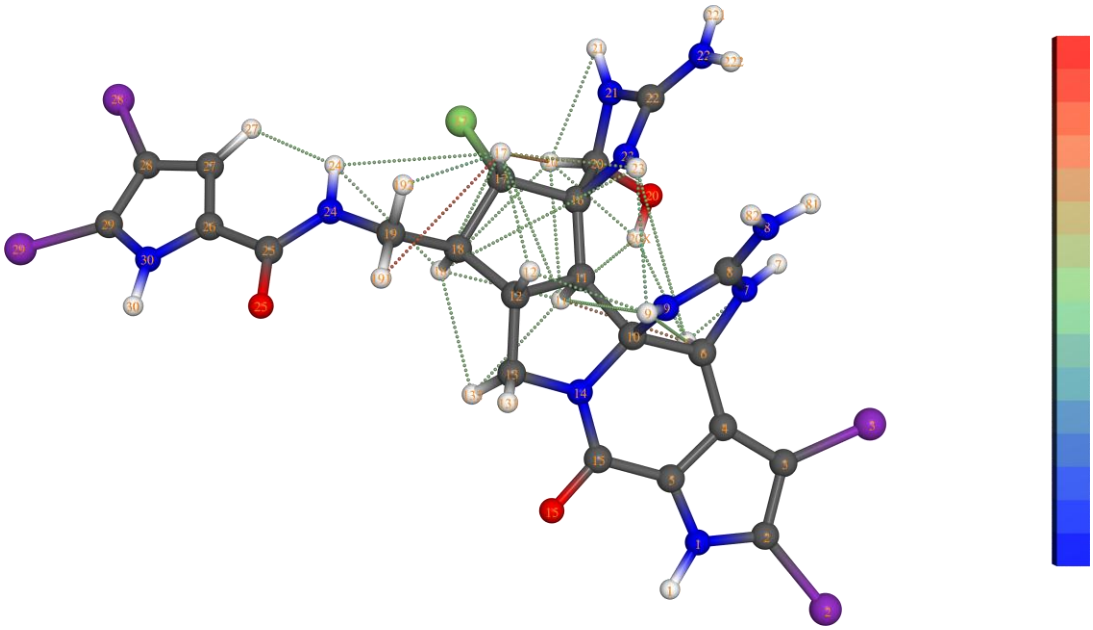


Figure S4. Plot of the best-fit (minimum pseudo energy) DG structure of Tetrabromostyloguanidine (**2**) with color-coded representation of all NOE contacts used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to +0.40 Å (red).

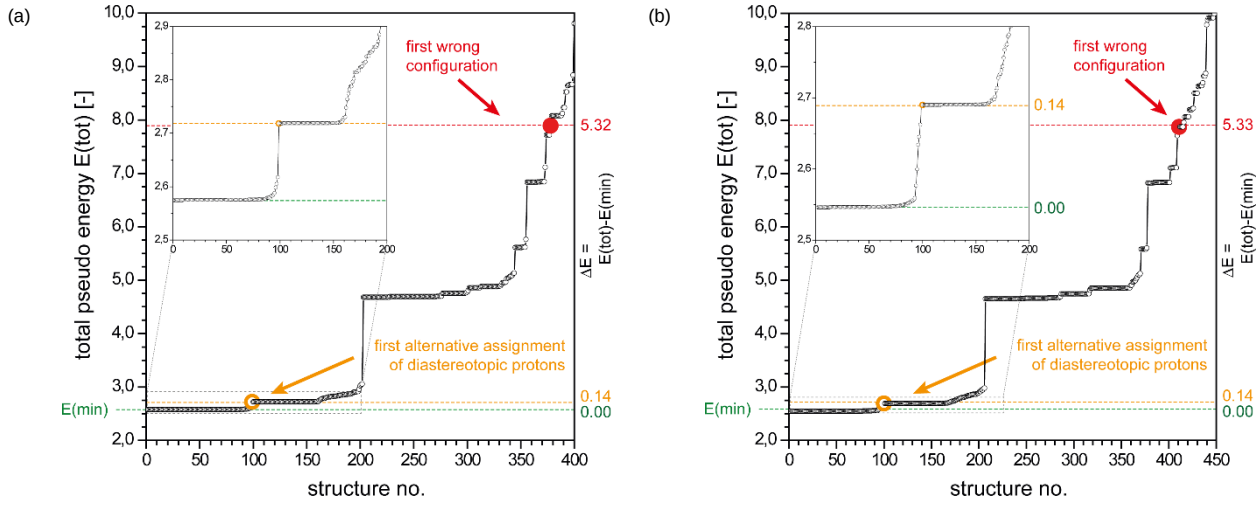
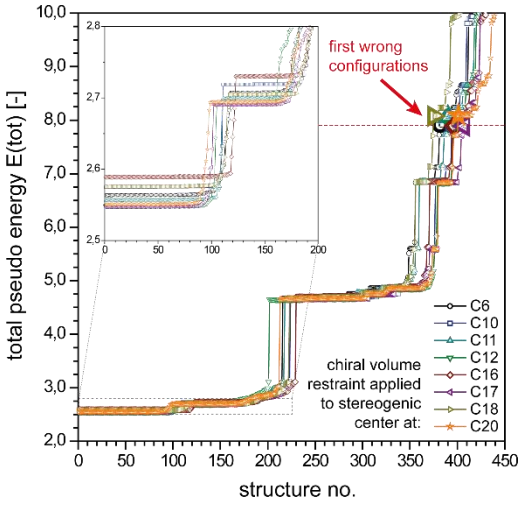


Figure S5.

(a) The *top left* plot shows pseudo energy sorted and ranked rDG structures of Tetrabromostyloguanidine (**2**) as discussed in the main paper. In this rDG simulation, a chiral volume restraint arbitrarily has been applied to a single stereogenic center (i.e. C10) in order to avoid enantiomeric structures.

(b) On the *top right*, the plot shows the corresponding pseudo energy of ranked rDG structures emerging from a simulation which did not use any chiral restraints at all, except on planar sp^2-type centers ($V_{chir} = 0$). The features of this plot, and in particular the energy steps are identical to the plot shown in (a), thus indicating that the arbitrary use of a single chiral volume restraint does not affect the final results of configurational and conformational analysis. In fact, this simulation produced the enantiomeric structures as shown below (Figure S6).

(c) On the *bottom right*, single chiral volume restraints were applied in rDG simulations on Tetrabromostyloguanidine (**2**), each using one of the eight stereogenic centers as a restrained and fixed reference. Restraining either one of C6, C10, C11, C12, C16, C17, C18, or C20 produces within very narrow margins of error the same energy step characteristics that have already been manifested in plots (a) and (b). In all cases, the first small step in energy results from an alternative assignment of diastereotopic methylene protons (see inset plot), and the first wrong relative configuration of one of the eight stereogenic centers (indicated by the bold-face large symbols) is always characterized by a significantly higher error in its total pseudo energy.



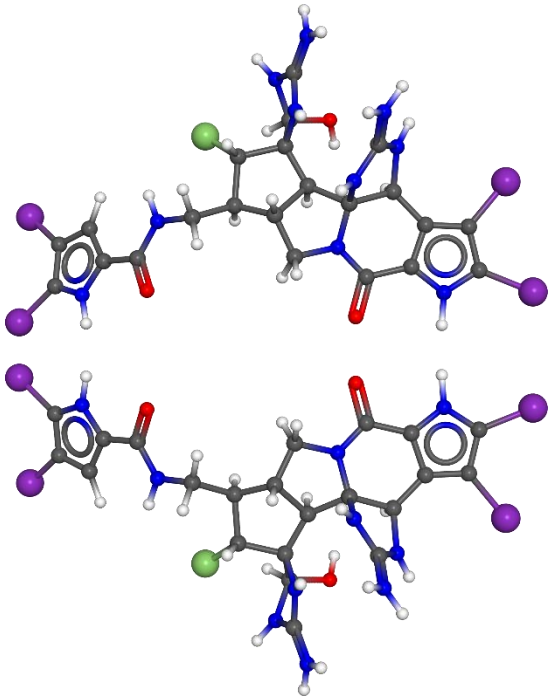
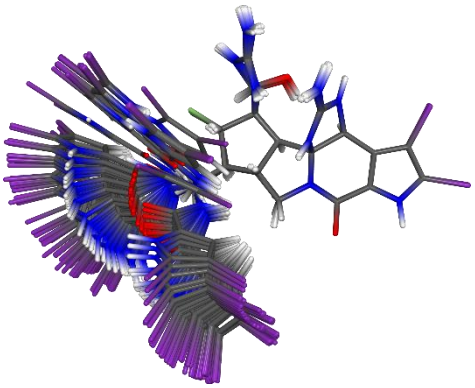
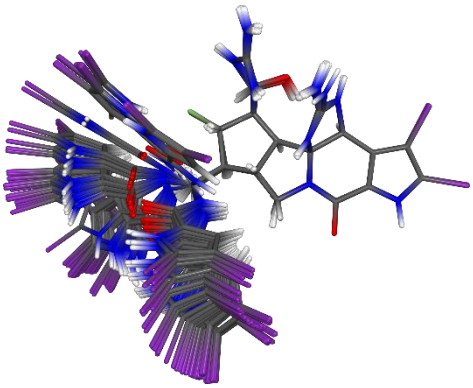


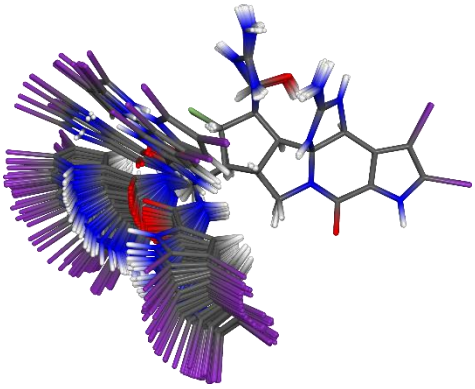
Figure S6. Ball-and-stick type representation of the first two lowest pseudo energy structures emerging from a rDG simulation on Tetrabromostyloguanidine (**2**) using no chiral restraints on any of the eight stereogenic centers, as shown in Figure S5b. These structures are actually exact enantiomers with identical pseudo energies.



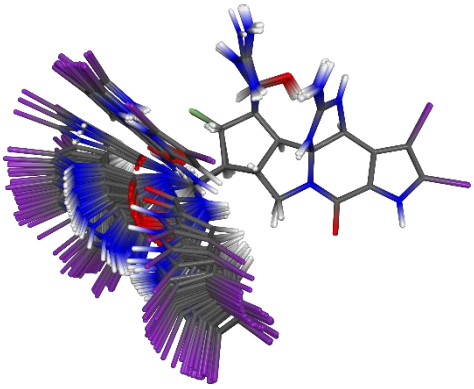
(a) chiral volume restraint applied to C6



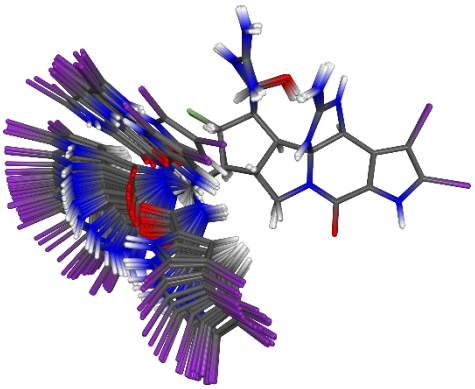
(b) chiral volume restraint applied to C10



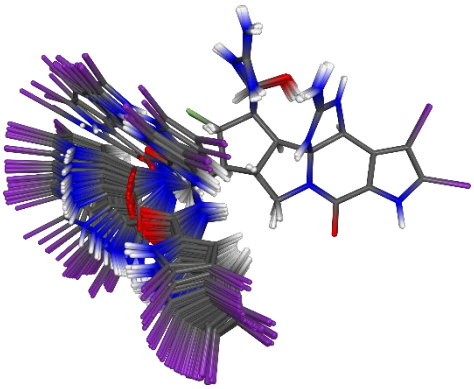
(c) chiral volume restraint applied to C11



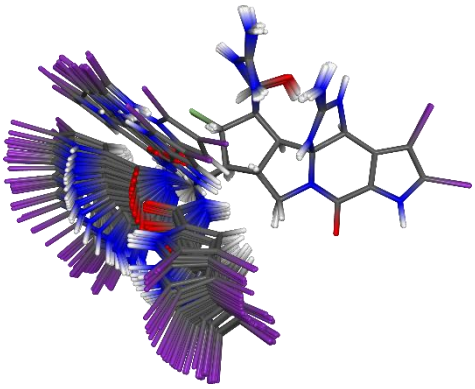
(d) chiral volume restraint applied to C12



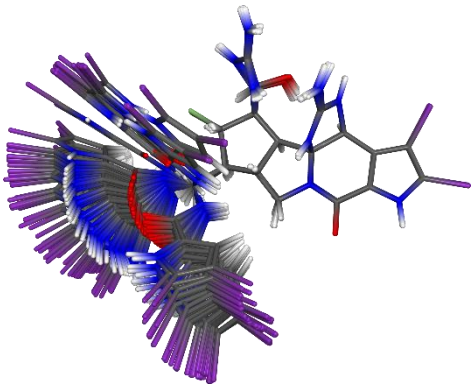
(e) chiral volume restraint applied to C16



(f) chiral volume restraint applied to C17



(g) chiral volume restraint applied to C18



(h) chiral volume restraint applied to C20

Figure S7. Ball-and-stick type representations of all low pseudo energy structures up to the first wrong configuration emerging from rDG simulations on Tetrabromostyloguanidine (**2**) using a single chiral volume restraints on one of the eight stereogenic centers, as shown in Figure S5c. All structures shown here actually feature the same configuration of all eight stereogenic centers (a: 381, b: 393, c: 389, d: 395, e: 396, f: 406, g: 374, and h: 400 structures in total).

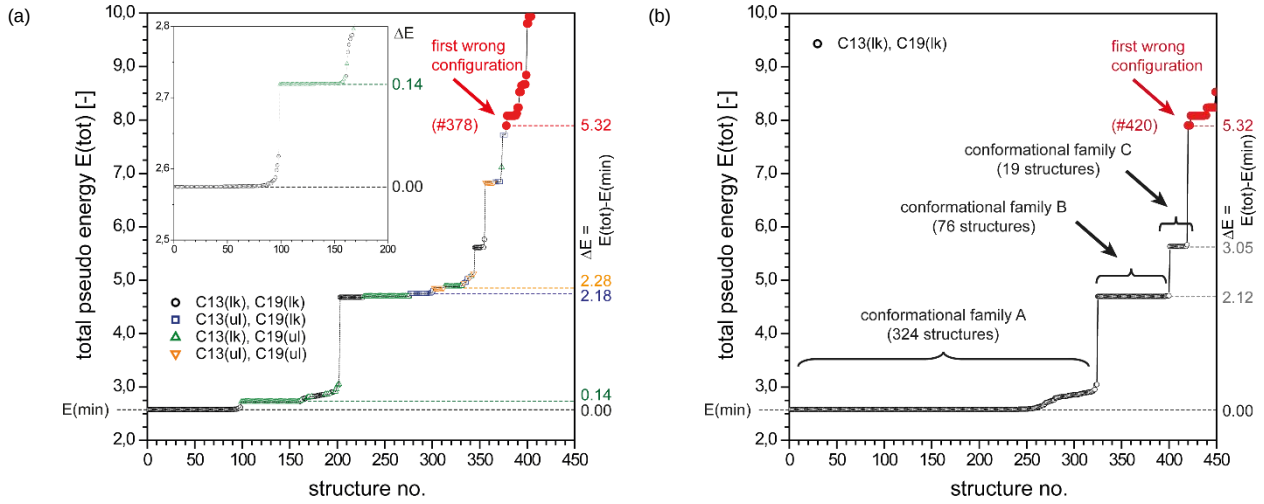
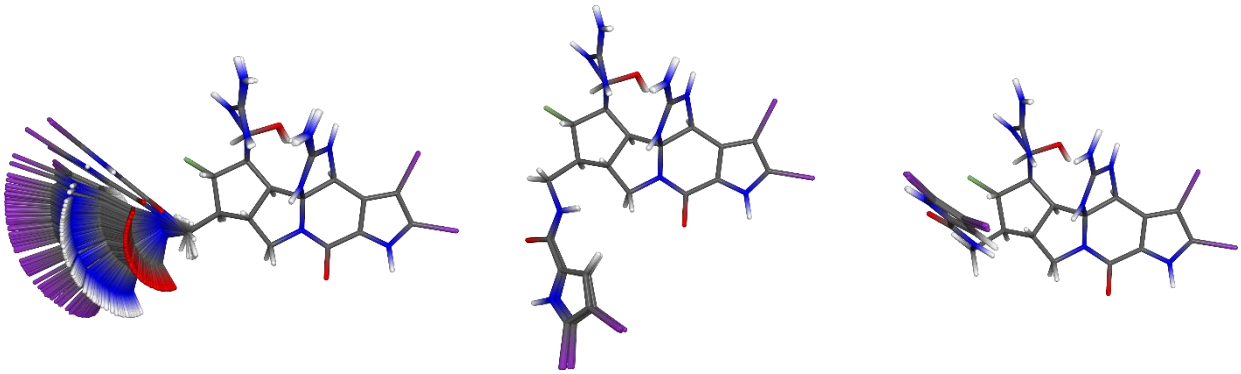


Figure S8. Detailed analysis of the assignments of diastereotopic methylene protons of Tetrabromostyloguanidine (**2**). (a) The *left plot* shows pseudo energy sorted and ranked rDG structures of **2** as discussed in the main paper. In addition, the color-coded symbols designate rankings of alternative assignments of CH2-protons (methylene groups C13 and C19), where the relative stereodescriptors "*lk*" (*like*) and "*ul*" (*unlike*) refer to the global pseudo energy minimum "*lk*/*lk*" assignment; the right scale gives ΔE values relative to $E(min)$. Different CH2-assignments were found (total number of structures generated: *lk*/*lk*: 162 (black), *ul*/*lk*: 44 (blue), *lk*/*ul*: 146 (green), and *ul*/*ul*: 25 (orange), with rankings of first occurrence *lk*/*lk*: #1 ($\Delta E = 0.00$), *ul*/*lk*: #277 ($\Delta E = 2.18$), *lk*/*ul*: #99 ($\Delta E = 0.14$), and *ul*/*ul*: #302 ($\Delta E = 2.28$)), which were ranked below the first wrong configuration of a stereogenic center (ranked no. #378, $\Delta E = 5.32$). (b) The *right plot* shows the pseudo energy of ranked rDG structures emerging from a simulation in which chiral volume restraints were used to restrict the pseudo configuration of both methylene groups in the correct low-energy configuration of plot (a). The sampling quality of correct *lk*/*lk* structures increases to 419 located below the occurrence of the first structure of wrong configuration ranked no. #420. The energy steps become significantly more pronounced as alternative assignments of methylene groups are discarded, and the low-energy structures cluster into three very distinct conformational families **A**-**C**. Below, superimposed structure plots of these different conformations are given (Figure S9).



conformational family **A** (324 structures) $\Delta E = 0.00$

conformational family **B** (76 structures) $\Delta E = 2.12$

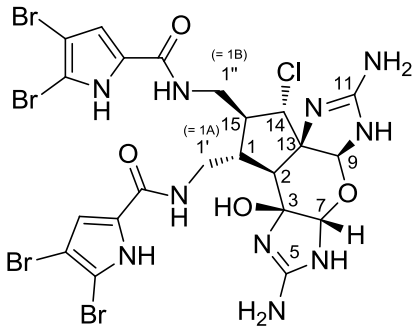
conformational family **C** (19 structures) $\Delta E = 3.05$

Figure S9. Superimposed structures for the conformational families **A**-**C** of Tetrabromostyloguanidine (**2**) as identified from the rDG simulation depicted in Figure S8b.

NOE and Structure Data for 3,7-*epi*-Massadine chloride (3)

Table S3. NOE data used for 3,7-*epi*-Massadine chloride (**3**) ($N = 37$ NOEs, the NMR-derived expectation values are denoted as d_{mean}, and the allowed lower and upper bonds – usually $d_{mean} \pm 10\%$ – are labeled as $d_{min} \cdots d_{max}$; the averaged distances back-calculated from structural data are labelled d_{calc}, and the corresponding residuals are listed only if this value falls out of range, i.e. $d_{calc} < d_{min}$ or $d_{calc} > d_{max}$; all distance are given in [Å]). The NOE labels refer to the formula shown on the right, where given as e.g. $H^A|H^B$, NOEs were recalculated from structures as r^{-6} averages over all pairs of atom-atom distances.

NOE		distances [Å]			
		d_{mean}	$d_{min} \cdots d_{max}$	d_{calc}	Δd
H3X	H7	3.316	2.984-3.648	3.068	-
H4	H1	4.164	3.748-4.580	3.738	-0.010
H4	H1A1	2.958	2.662-3.253	3.354	0.101
H4	H1A2	3.416	3.074-3.758	3.783	0.025
H4	H2	3.014	2.712-3.315	3.294	-
H4	H7	2.710	2.439-2.981	3.208	0.227
H7	H1	4.709	4.238-5.179	4.582	-
H7	H2	3.574	3.216-3.931	3.834	-
H9	H1	5.200	4.680-5.719	5.133	-
H9	H15	6.381	5.743-7.019	5.383	-0.360
H9	H2	2.906	2.615-3.197	3.238	0.041
H9	H7	3.559	3.204-3.915	3.804	-
H12	H1	2.568	2.311-2.825	2.213	-0.098
H12	H14	3.200	2.880-3.520	3.238	-
H12	H15	3.255	2.929-3.580	3.900	0.320
H12	H1B1	3.077	2.770-3.385	2.673	-0.097
H12	H1B2	3.812	3.431-4.193	3.717	-
H12	H2	3.377	3.039-3.714	3.792	0.078
H12	H7	3.566	3.209-3.923	4.005	0.082
H12	H9	4.641	4.177-5.105	4.225	-
H14	H1	3.398	3.058-3.739	3.873	0.134
H14	H15	2.951	2.656-3.246	2.817	-
H14	H1B1	2.839	2.555-3.123	2.468	-0.087
H14	H1B2	3.342	3.008-3.676	3.434	-
H14	H2	3.519	3.168-3.871	3.778	-
H1A1	H1	2.650	2.385-2.915	2.321	-0.064
H1A1	H15	2.821	2.539-3.103	3.424	0.321
H1A1	H1A2	1.780	1.602-1.958	1.817	-
H1A1	H2	3.218	2.897-3.540	3.463	-
H1A2	H1	2.722	2.450-2.994	3.067	0.073
H1A2	H15	3.054	2.748-3.360	2.892	-
H1A2	H2	2.949	2.654-3.244	2.522	-0.132
H1B1	H1	2.776	2.499-3.054	3.255	0.201
H1B1	H15	2.893	2.603-3.182	2.943	-
H1B2	H1	2.742	2.467-3.016	3.125	0.109
H1B2	H15	2.492	2.243-2.741	2.174	-0.069
H1B2	H1B1	2.002	1.801-2.202	1.777	-0.024



3,7-*epi*-Massadine chloride (**3**)

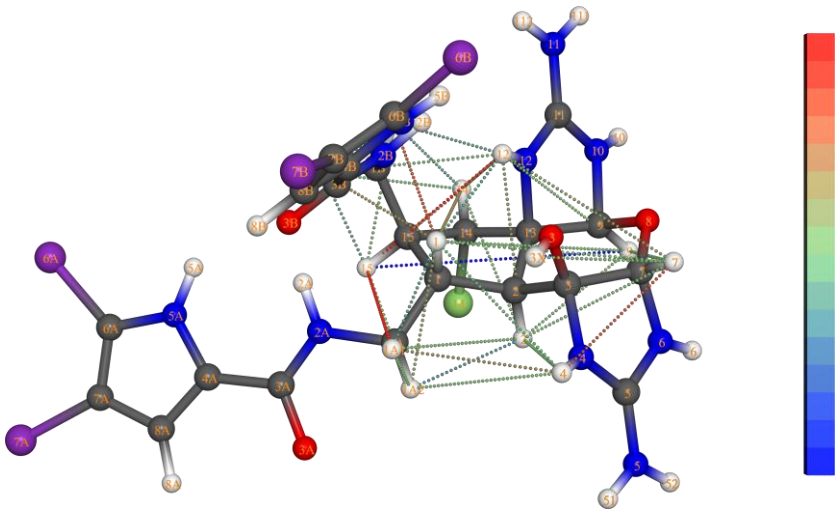


Figure S10. Plot of the best-fit (minimum pseudo energy) DG structure of 3,7-*epi*-Massadine chloride (**3**) with color-coded representation of all NOE contacts used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to +0.40 Å (red).

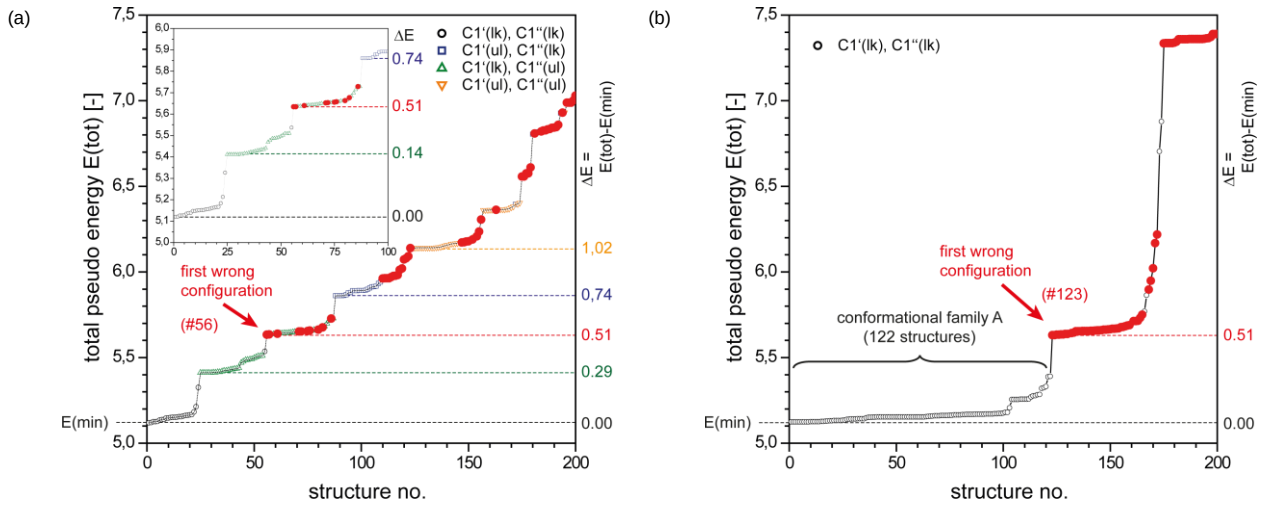
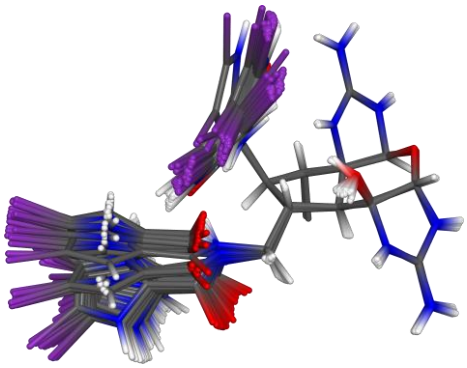


Figure S11. Detailed analysis of the assignments of diastereotopic methylene protons of 3,7-*epi*-Massadine chloride (**3**). (a) The *left plot* shows pseudo energy sorted and ranked rDG structures of **3** as discussed in the main paper. In addition, the color-coded symbols designate rankings of alternative assignments of CH2-protons (methylene groups C1' and C1''), where the relative stereodescriptors "*lk*" (*like*) and "*ul*" (*unlike*) refer to the global pseudo energy minimum "*lk*/*lk*" assignment; the right scale gives ΔE values relative to $E(min)$. Different CH2-assignments were found (total number of structures generated: *lk*/*lk*: 25 (black), *ul*/*lk*: 0 (blue), *lk*/*ul*: 30 (green), and *ul*/*ul*: 0 (orange), with rankings of first occurrence *lk*/*lk*: #1 ($\Delta E = 0.00$), *ul*/*lk*: #88 ($\Delta E = 0.74$), *lk*/*ul*: #25 ($\Delta E = 0.29$), and *ul*/*ul*: #124 ($\Delta E = 1.02$)), which were ranked below the first wrong configuration of a stereogenic center (ranked no. #56, $\Delta E = 0.51$). (b) The *right plot* shows the pseudo energy of ranked rDG structures emerging from a simulation in which chiral volume restraints were used to restrict the pseudo configuration of both methylene groups in the correct low-energy configuration of plot (a). The sampling quality of correct *lk*/*lk* structures increases to 122 located below the occurrence of the first structure of wrong configuration ranked no. #123. The energy steps become significantly more pronounced as alternative assignments of methylene groups are discarded, and the low-energy structures cluster into a single conformational family **A**. Below, a plot of these superimposed structures is given (Figure S12).



conformational family **A** (122 structures)
$\Delta E = 0.00$

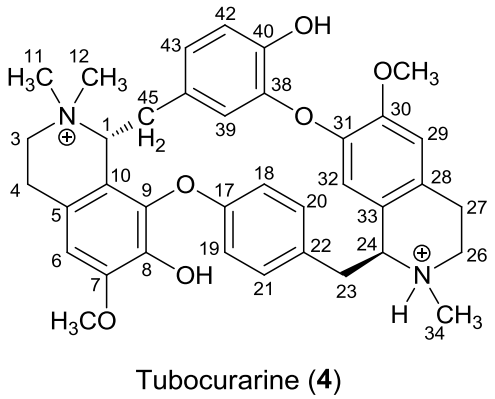
Figure S12. Superimposed structures for the main low-pseudo energy conformational family **A** of 3,7-*epi*-Massadine chloride (**3**) as identified from the rDG simulation depicted in Figure S11b.

NOE, RDC, and Structure Data for Tubocurarine (4)

The following table provides data on the RDCs (D^{exp}) used for Tubocurarine (**4**, three alignment media labeled [A]-[C]), their back-calculated values (D^{calc}), and residuals ($\Delta D = D^{exp} - D^{calc}$).

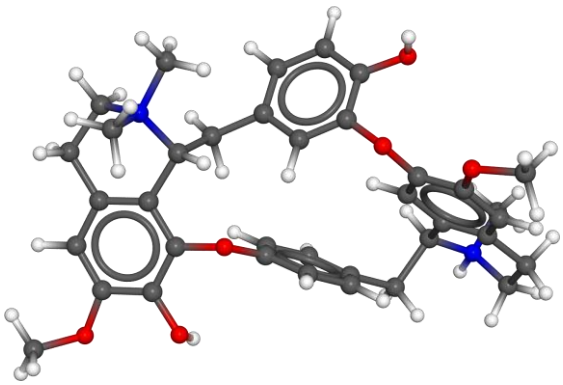
Table S4. RDC data used for Tubocurarine (**4**) ($N = 16$ RDCs, best-fit back-calculated RDCs D^{calc} for each alignment medium (AM) labeled [A], [B], and [C], and residuals $\Delta D = D^{exp} - D^{calc}$, all values in [Hz]). Only bold face entries were used as parameters for the RDC analysis, regular font entries designate the calculated split terms of compound RDCs (where applicable, sums of RDCs are denoted as C-H^A+C-H^B = $D(CH^A) + D(CH^B)$, averages of RDCs are denoted as C-H^A|C-H^B = $(D(CH^A) + D(CH^B))/2$, methyl-RDCs were considered as three-state averages C-H^A|H^B|H^C); the RDC labels refer to the formula shown on the right).

RDC	AM [A]			AM [B]			AM [C]		
	D^{exp}	D^{calc}	ΔD	D^{exp}	D^{calc}	ΔD	D^{exp}	D^{calc}	ΔD
C1-H1	**-9.13**	**-9.17**	**0.04**	**-4.33**	**-4.37**	**0.04**	**-0.04**	**-0.12**	**0.08**
C3-H3A+C3-H3B	**2.18**	**2.16**	**0.02**	**-11.53**	**-11.51**	**-0.02**	**24.69**	**24.68**	**0.01**
C3-H3A	-	-23.29	-	-	-18.27	-	-	19.61	-
C3-H3B	-	25.45	-	-	6.76	-	-	5.07	-
C4-H4A+C4-H4B	**19.99**	**19.98**	**0.01**	**6.87**	**6.89**	**-0.02**	**1.42**	**1.43**	**-0.01**
C4-H4A	-	14.53	-	-	7.09	-	-	14.14	-
C4-H4B	-	5.45	-	-	-0.20	-	-	-12.71	-
C6-H6	**-19.54**	**-19.57**	**0.03**	**8.00**	**8.04**	**-0.04**	**9.06**	**9.06**	**0.00**
C18-H18|C19-H19	**-1.09**	**-1.15**	**0.06**	**-3.48**	**-3.50**	**0.02**	**4.76**	**4.68**	**0.08**
C18-H18	-	23.98	-	-	0.51	-	-	-6.11	-
C19-H19	-	-26.28	-	-	-7.50	-	-	15.47	-
C20-H20|C21-H21	**-1.55**	**-1.53**	**-0.02**	**-4.52**	**-4.37**	**-0.15**	**3.19**	**3.31**	**-0.12**
C20-H20	-	-25.58	-	-	-8.69	-	-	15.22	-
C21-H21	-	22.52	-	-	-0.04	-	-	-8.60	-
C23-H23A+C23-H23B	**-4.67**	**-4.66**	**-0.01**	**-16.38**	**-16.40**	**0.02**	**-5.03**	**-5.05**	**0.02**
C23-H23A	-	-23.42	-	-	-18.64	-	-	19.00	-
C23-H23B	-	18.77	-	-	2.24	-	-	-24.04	-
C24-H24	**-24.11**	**-24.09**	**-0.02**	**-18.45**	**-18.59**	**0.14**	**19.33**	**19.33**	**0.00**
C26-H26A+C26-H26B	**7.52**	**7.48**	**0.04**	**10.11**	**10.16**	**-0.05**	**12.14**	**12.10**	**0.04**
C26-H26A	-	-6.30	-	-	0.75	-	-	24.81	-
C26-H26B	-	13.79	-	-	9.41	-	-	-12.71	-
C27-H27A+C27-H27B	**1.62**	**1.66**	**-0.04**	**3.54**	**3.61**	**-0.07**	**2.29**	**2.35**	**-0.06**
C27-H27A	-	-13.50	-	-	-15.79	-	-	13.38	-
C27-H27B	-	15.16	-	-	19.40	-	-	-11.03	-
C29-H29	**-23.06**	**-22.88**	**-0.18**	**-2.94**	**-2.83**	**-0.11**	**10.20**	**10.37**	**-0.17**
C32-H32	**-22.20**	**-22.48**	**0.28**	**-3.65**	**-3.63**	**-0.02**	**10.36**	**10.15**	**0.21**
C39-H39	**12.20**	**12.33**	**-0.13**	**2.24**	**2.04**	**0.20**	**-3.98**	**-4.11**	**0.13**
C42-H42	**11.53**	**11.31**	**0.22**	**0.62**	**0.84**	**-0.22**	**-3.70**	**-3.63**	**-0.07**
C43-H43	**-24.30**	**-24.19**	**-0.11**	**-14.21**	**-14.32**	**0.11**	**17.12**	**17.14**	**-0.02**
C45-H45A+C45-H45B	**-22.14**	**-22.21**	**0.07**	**-26.90**	**-26.74**	**-0.16**	**6.48**	**6.48**	**0.00**
C45-H45A	-	-11.01	-	-	-15.26	-	-	-2.03	-
C45-H45B	-	-11.20	-	-	-11.47	-	-	8.51	-



Tubocurarine (**4**)

Figure S13. Plot of the experimental RDCs (D^{exp}) vs. their back-calculated values (D^{calc}) used for Tubocurarine (**4**, three alignment media labeled [A]-[C]). The corresponding best-fit (lowest total *pseudo energy*) structure model (see plot below) was obtained from the DG simulation using all three AM data sets.



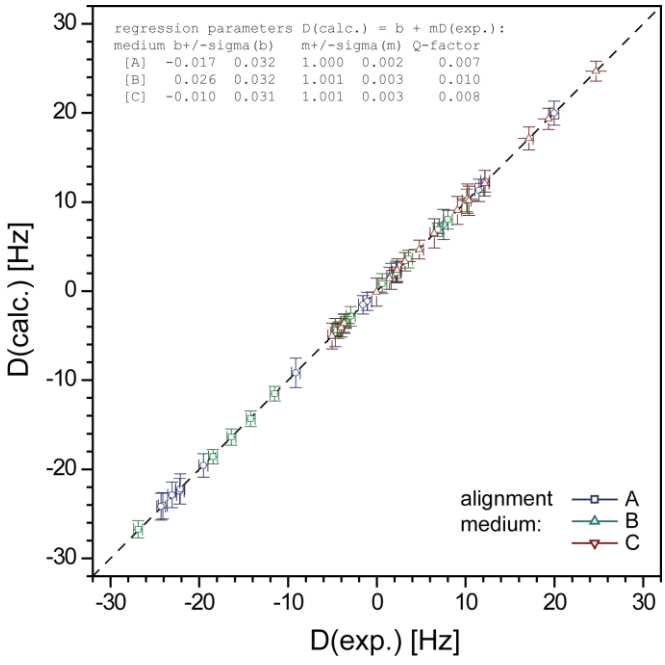
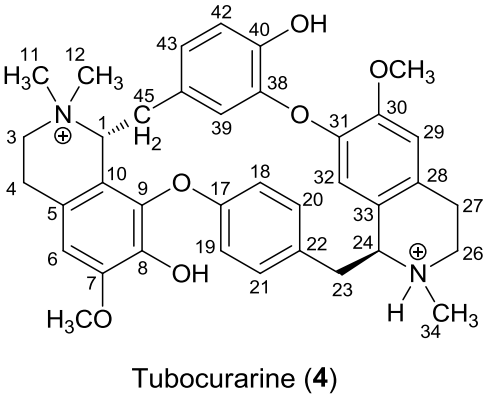


Table S5. NOE data used for Tubocurarine (**4**) ($N = 17$ NOEs, the NMR-derived expectation values are denoted as d_{mean}, and the allowed lower and upper bonds – usually $d_{mean} \pm 10\%$ – are labeled as $d_{min} \cdots d_{max}$; the averaged distances back-calculated from structural data are labelled d_{calc}, and the corresponding residuals are listed only if this value falls out of range, i.e. $d_{calc} < d_{min}$ or $d_{calc} > d_{max}$; all distance are given in [Å]). The NOE labels refer to the formula shown on the right, where given as e.g. $H^A|H^B$, NOEs were recalculated from structures as r^{-6} averages over all pairs of atom-atom distances.

NOE		distances [Å]			
		d_{mean}	$d_{min} \cdots d_{max}$	d_{calc}	Δd
H1	H39	2.166	1.949-2.383	2.300	-
H1	H45A|H45B	2.639	2.375-2.903	2.654	-
H3A|H3B	H4A|H4B	2.473	2.226-2.720	2.488	-
H4A|H4B	H6	2.690	2.421-2.959	2.724	-
H6	H14A|H14B|H14C	2.476	2.228-2.724	2.414	-
H18|H19	H39	3.414	3.073-3.755	3.131	-
H18|H19	H45A|H45B	2.525	2.272-2.778	2.548	-
H20|H21	H23A|H23B	2.646	2.381-2.911	2.767	-
H20|H21	H24	3.279	2.951-3.607	3.289	-
H23A|H23B	H24	3.024	2.722-3.326	2.663	-0.059
H23A|H23B	H26A|H26B	2.336	2.102-2.570	2.561	-
H24	H32	2.338	2.104-2.572	2.385	-
H26A|H26B	H27A|H27B	2.438	2.194-2.682	2.480	-
H27A|H27B	H29	2.669	2.402-2.936	2.701	-
H29	H36A|H36B|H36C	2.365	2.129-2.602	2.347	-
H39	H45A|H45B	2.972	2.675-3.269	2.879	-
H43	H45A|H45B	3.287	2.958-3.616	2.730	-0.228



Tubocurarine (**4**)

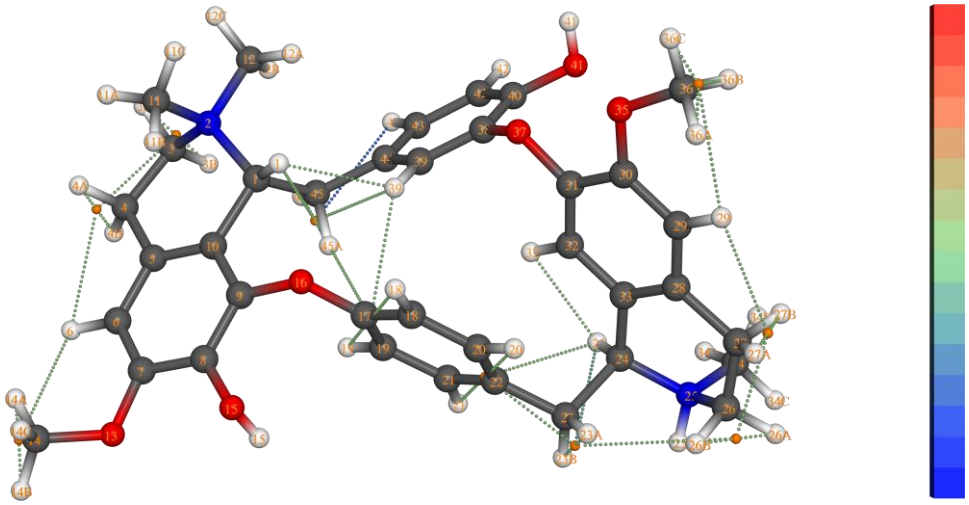


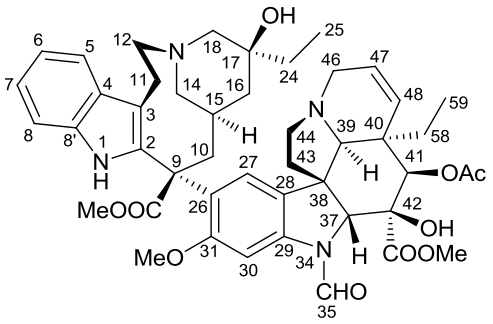
Figure S14. Plot of the best-fit (minimum pseudo energy) DG structure of Tubocurarine (**4**) with color-coded representation of all NOE contacts used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to +0.40 Å (red).

NOE, RDC, and Structure Data for Vincristine (5)

The following table provides data on the RDCs (D^{exp}) used for Vincristine (**5**, three alignment media labeled [A]-[C]), their back-calculated values (D^{calc}), and residuals ($\Delta D = D^{exp} - D^{calc}$).

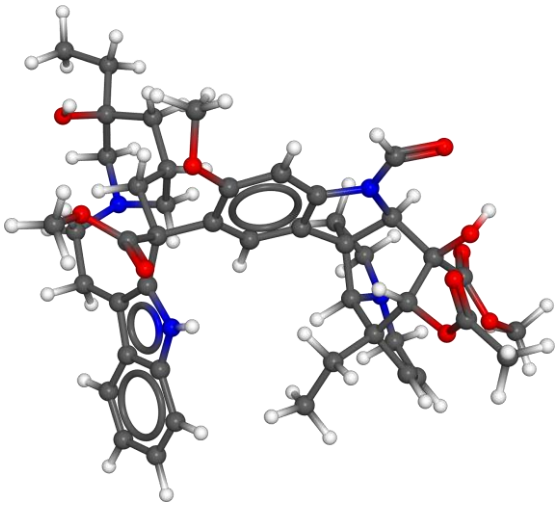
Table S6. RDC data used for Vincristine (**5**) ($N = 24$ RDCs, best-fit back-calculated RDCs D^{calc} for each alignment medium (AM) labeled [A], [B], and [C], and residuals $\Delta D = D^{exp} - D^{calc}$, all values in [Hz]). Only bold face entries were used as parameters for the RDC analysis, regular font entries designate the calculated split terms of compound RDCs (where applicable, sums of RDCs are denoted as C-H^A+C-H^B = $D(CH^A) + D(CH^B)$, averages of RDCs are denoted as C-H^A|C-H^B = $(D(CH^A) + D(CH^B))/2$, methyl-RDCs were considered as three-state averages C-H^A|H^B|H^C); the RDC labels refer to the formula shown on the right).

RDC	AM [A]			AM [B]			AM [C]		
	D^{exp}	D^{calc}	ΔD	D^{exp}	D^{calc}	ΔD	D^{exp}	D^{calc}	ΔD
C5-H5	**18.60**	**18.68**	**-0.08**	**-25.15**	**-25.28**	**0.13**	**4.92**	**5.16**	**-0.24**
C6-H6	**4.47**	**4.49**	**-0.02**	**20.86**	**20.87**	**-0.01**	**19.24**	**19.33**	**-0.09**
C7-H7	**-0.13**	**-0.14**	**0.01**	**10.27**	**10.24**	**0.03**	**12.44**	**12.50**	**-0.06**
C8-H8	**19.98**	**19.92**	**0.06**	**-24.19**	**-24.18**	**-0.01**	**5.26**	**5.19**	**0.07**
C10-H10A+C10-H10B	**-4.79**	**-4.80**	**0.01**	**0.49**	**0.49**	**0.00**	**15.57**	**15.52**	**0.05**
C10-H10A	-	-16.23	-	-	-22.31	-	-	-0.54	-
C10-H10B	-	11.43	-	-	22.79	-	-	16.07	-
C11-H11A+C11-H11B	**-8.62**	**-8.65**	**0.03**	**8.17**	**8.20**	**-0.03**	**-18.08**	**-18.08**	**0.00**
C11-H11A	-	-27.51	-	-	-6.36	-	-	-18.44	-
C11-H11B	-	18.85	-	-	14.56	-	-	0.36	-
C12-H12A+C12-H12B	**29.22**	**29.20**	**0.02**	**-10.72**	**-10.65**	**-0.07**	**5.25**	**5.19**	**0.06**
C12-H12A	-	16.79	-	-	13.76	-	-	-1.84	-
C12-H12B	-	12.41	-	-	-24.41	-	-	7.03	-
C14-H14A+C14-H14B	**-13.51**	**-13.51**	**0.00**	**10.35**	**10.35**	**0.00**	**-11.89**	**-11.88**	**-0.01**
C14-H14A	-	-14.07	-	-	1.75	-	-	-22.71	-
C14-H14B	-	0.56	-	-	8.60	-	-	10.83	-
C15-H15	**-8.57**	**-8.57**	**0.00**	**-27.71**	**-27.68**	**-0.03**	**1.00**	**0.98**	**0.02**
C16-H16A+C16-H16B	**-3.06**	**-3.07**	**0.01**	**17.72**	**17.74**	**-0.02**	**-16.21**	**-16.22**	**0.01**
C16-H16A	-	18.92	-	-	16.34	-	-	3.92	-
C16-H16B	-	-21.99	-	-	1.40	-	-	-20.14	-
C18-H18A+C18-H18B	**-17.52**	**-17.52**	**0.00**	**-25.70**	**-25.70**	**0.00**	**-20.39**	**-20.38**	**-0.01**
C18-H18A	-	-12.45	-	-	0.78	-	-	-23.66	-
C18-H18B	-	-5.07	-	-	-26.48	-	-	3.28	-
C24-H24A+C24-H24B	**0.94**	**0.94**	**0.00**	**15.75**	**15.75**	**0.00**	**-9.08**	**-9.09**	**0.01**
C24-H24A	-	13.46	-	-	20.27	-	-	15.55	-
C24-H24B	-	-12.51	-	-	-4.51	-	-	-24.64	-
C27-H27	**14.52**	**14.49**	**0.03**	**18.78**	**18.67**	**0.11**	**15.29**	**15.24**	**0.05**
C30-H30	**17.02**	**17.00**	**0.02**	**14.74**	**14.84**	**-0.10**	**14.06**	**14.14**	**-0.08**
C35-H35	**7.91**	**8.01**	**-0.10**	**6.56**	**6.36**	**0.20**	**-11.24**	**-11.17**	**-0.07**
C37-H37	**-16.61**	**-16.63**	**0.02**	**8.66**	**8.65**	**0.01**	**-15.02**	**-14.97**	**-0.05**
C39-H39	**-24.87**	**-24.93**	**0.06**	**2.00**	**1.90**	**0.10**	**4.18**	**4.31**	**-0.13**
C41-H41	**-5.03**	**-5.03**	**0.00**	**-4.67**	**-4.65**	**-0.02**	**-19.53**	**-19.49**	**-0.04**
C43-H43A+C43-H43B	**-30.83**	**-30.77**	**-0.06**	**3.45**	**3.46**	**-0.01**	**13.99**	**13.95**	**0.04**
C43-H43A	-	-16.03	-	-	-24.48	-	-	-1.86	-
C43-H43B	-	-14.74	-	-	27.94	-	-	15.81	-
C44-H44A+C44-H44B	**-14.42**	**-14.41**	**-0.01**	**6.81**	**6.79**	**0.02**	**2.47**	**2.45**	**0.02**
C44-H44A	-	14.27	-	-	2.35	-	-	14.36	-
C44-H44B	-	-28.68	-	-	4.44	-	-	-11.91	-
C46-H46A+C46-H46B	**-22.40**	**-22.40**	**0.00**	**-2.47**	**-2.48**	**0.01**	**-10.39**	**-10.39**	**0.00**
C46-H46A	-	-16.83	-	-	-0.89	-	-	-23.50	-
C46-H46B	-	-5.57	-	-	-1.59	-	-	13.11	-
C47-H47	**-0.88**	**-0.95**	**0.07**	**-3.29**	**-3.27**	**-0.02**	**-0.91**	**-0.89**	**-0.02**
C48-H48	**15.49**	**15.47**	**0.02**	**-13.54**	**-13.56**	**0.02**	**3.53**	**3.48**	**0.05**
C58-H58A+C58-H58B	**22.26**	**22.26**	**0.00**	**-24.94**	**-24.94**	**0.00**	**-2.45**	**-2.44**	**-0.01**
C58-H58A	-	25.15	-	-	-16.08	-	-	1.17	-
C58-H58B	-	-2.89	-	-	-8.86	-	-	-3.61	-



Vincristine (**5**)

Figure S15. Plot of the experimental RDCs (D^{exp}) vs. their back-calculated values (D^{calc}) used for Vincrsitine (**5**, three alignment media labeled [A]-[C]). The corresponding best-fit (lowest total *pseudo energy*) structure model (see plot below) was obtained from the DG simulation using all three AM data sets.



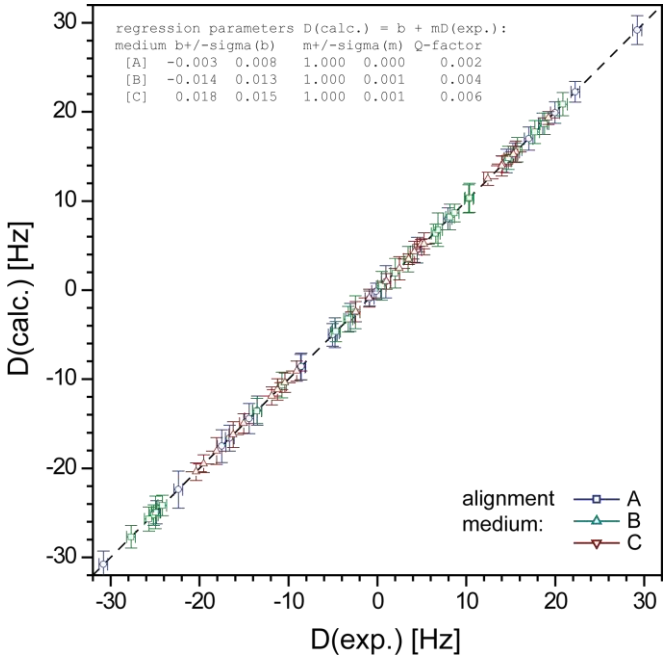
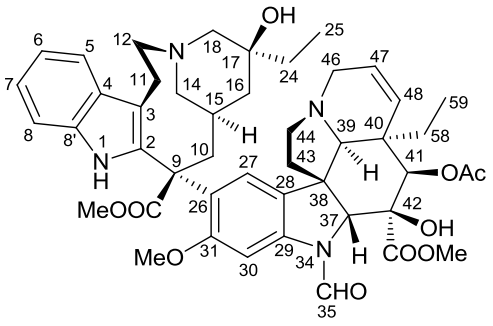


Table S7. NOE data used for Vincristine (**5**) ($N = 23$ NOEs, the NMR-derived expectation values are denoted as d_{mean}, and the allowed lower and upper bonds – usually $d_{mean} \pm 10\%$ – are labeled as $d_{min} \cdots d_{max}$; the averaged distances back-calculated from structural data are labelled d_{calc}, and the corresponding residuals are listed only if this value falls out of range, i.e. $d_{calc} < d_{min}$ or $d_{calc} > d_{max}$; all distance are given in [Å]). The NOE labels refer to the formula shown on the right, where given as e.g. $H^A|H^B$, NOEs were recalculated from structures as r^{-6} averages over all pairs of atom-atom distances.

NOE		distances [Å]			
		d_{mean}	$d_{min} \cdots d_{max}$	d_{calc}	Δd
H30	H35	2.206	1.985-2.426	2.149	-
H27	H39	2.458	2.212-2.704	2.565	-
H1	H27	2.672	2.405-2.939	2.877	-
H15	H27	2.684	2.416-2.952	2.752	-
H10A|H10B	H12A|H12B	2.176	1.958-2.394	2.290	-
H10A|H10B	H16A|H16B	2.783	2.505-3.061	2.809	-
H12A|H12B	H18A|H18B	2.705	2.435-2.976	2.703	-
H14A|H14B	H16A|H16B	3.100	2.790-3.410	3.162	-
H14A|H14B	H18A|H18B	2.926	2.633-3.219	2.940	-
H14A|H14B	H27	2.598	2.338-2.858	2.621	-
H16A|H16B	H18A|H18B	3.292	2.963-3.621	3.310	-
H27	H43A|H43B	2.894	2.605-3.183	2.725	-
H27	H58A|H58B	3.304	2.974-3.634	3.563	-
H37	H43A|H43B	2.562	2.306-2.818	2.533	-
H37	H44A|H44B	3.287	2.958-3.616	3.319	-
H39	H41	3.463	3.117-3.809	3.448	-
H39	H43A|H43B	3.140	2.826-3.454	3.190	-
H39	H44A|H44B	3.330	2.997-3.663	3.415	-
H39	H46A|H46B	3.014	2.713-3.315	3.091	-
H39	H58A|H58B	2.653	2.388-2.918	2.611	-
H41	H58A|H58B	2.361	2.125-2.597	2.369	-
H44A|H44B	H46A|H46B	2.829	2.546-3.112	2.798	-
H48	H58A|H58B	2.864	2.578-3.150	2.946	-



Vincristine (**5**)

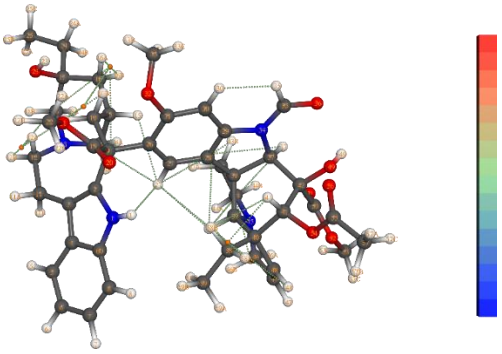


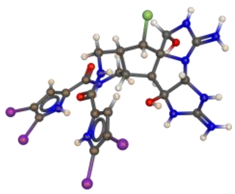
Figure S16. Plot of the best-fit (minimum pseudo energy) DG structure of Vincrsitine (**5**) with color-coded representation of all NOE contacts used in the configurational and conformational analysis. The color scale was adapted from calculated final NOE violations, ranging from -0.40 Å (blue) to +0.40 Å (red).

Atomic Coordinates for Compounds (1)-(5)

The following tables provide the atomic coordinates for the final best-fit (minimum pseudo energy) DG structures of (**1**)-(**5**), copy-and-paste for further usage:

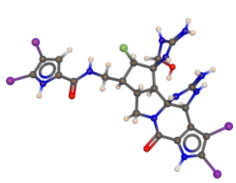
Table S8. rDG best-fit structures (atomic coordinates) for compounds (**1**)-(**5**).

Axinellamine A (1)



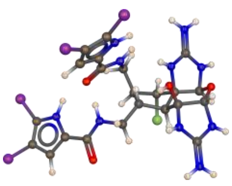
Axinellamine A (1)			
C1	-2.881472	-0.668349	-2.430370
O1	-2.981222	0.523986	-3.235802
N2	-4.324663	-0.969276	-2.138918
C3	-4.549924	-0.249399	-0.892619
N3	-5.768046	-0.295439	-0.449255
N4	-3.502670	0.325330	-0.422748
C5	-3.196253	0.748263	0.886095
N6	-3.749854	2.034221	1.453231
C7	-2.885993	2.998609	1.166591
N7	-3.171249	4.301521	1.111965
N8	-1.555804	2.541736	0.892792
C9	-1.646724	1.136881	0.798655
O9	-0.939405	0.557697	1.882486
C10	-1.248805	0.450979	-0.572135
C11	0.116996	-0.267510	-0.813149
C12	-0.331439	-1.821680	-0.875671
C13	-1.817884	-1.816823	-0.377278
C14	-2.288783	-0.464970	-1.021748
Cl13	-2.831937	-3.200003	-0.884687
H1	-2.453310	-1.437547	-3.073108
H1X	-2.120933	0.924197	-3.188836
H2	-4.874481	-1.424519	-2.561413
H5	-3.338464	-0.048025	1.616712
H6	-4.620894	2.074139	1.964952
H8	-0.852556	3.125308	0.811365
H9X	-1.469501	0.547905	2.630721
H10	-1.071173	1.356981	-1.151538
H11	0.698458	-0.136580	0.099463
H12	-0.217453	-2.143055	-1.910961
H13	-1.837498	-1.791260	0.712246
H31	-6.512999	-0.856523	-1.027783
H32	-6.077495	0.173576	0.426819
H71	-4.111660	4.681821	1.293034
H72	-2.353895	4.969231	0.855326
C1A	0.606415	-2.779441	-0.020340
N2A	0.752941	-2.217826	1.345091
C3A	1.821056	-1.409536	1.679714
O3A	2.707677	-1.089074	0.880762
C4A	1.804362	-0.961023	3.098397
N5A	2.747961	-0.145214	3.712314
C6A	2.416978	0.064389	5.029910
C7A	1.228437	-0.635919	5.269095
C8A	0.835502	-1.282860	4.063682
Br6A	3.433965	1.116688	6.227979
Br7A	0.249332	-0.752861	6.890224
H1A1	0.205893	-3.790653	0.051292
H1A2	1.590515	-2.683714	-0.479126
H2A	0.079800	-2.443317	2.068857
H5A	3.597427	0.254302	3.230033
H8A	-0.049253	-1.905327	3.930105
C1B	0.769119	0.212176	-2.160517
N2B	2.232033	0.246003	-2.021631
C3B	3.079549	0.220478	-3.091402
O3B	2.697079	0.167026	-4.272778
C4B	4.519527	0.262689	-2.711158
N5B	5.023270	0.322780	-1.418525
C6B	6.398470	0.348101	-1.440378
C7B	6.785626	0.302897	-2.786256
C8B	5.614824	0.249234	-3.589868
Br6B	7.483614	0.429131	0.105064
Br7B	8.546853	0.308894	-3.492731
H1B1	0.478137	1.240751	-2.373739
H1B2	0.515556	-0.447754	-2.990154
H2B	2.572969	0.288307	-1.090752
H5B	4.432486	0.345702	-0.544018
H8B	5.587314	0.206211	-4.678671

Tetrabromostylo-guanidine (2)



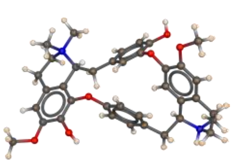
Tetrabromostylo-guanidine (2)			
N1	-5.497115	-2.659226	-0.082654
C2	-6.538583	-1.858724	-0.374497
C3	-6.048074	-0.554340	-0.726067
C4	-4.654755	-0.637226	-0.626045
C5	-4.355385	-1.965678	-0.220149
C6	-3.505014	0.282697	-0.819907
N7	-3.381257	1.516311	-1.613506
C8	-2.574322	1.118146	-2.678949
N8	-2.433313	1.772453	-3.799864
N9	-1.947657	-0.089088	-2.346162
C10	-2.097230	-0.317940	-0.895695
C11	-0.819644	0.309681	-0.284862
C12	0.219656	-0.918148	-0.599948
C13	-0.564104	-2.116785	-0.270724
N14	-1.938463	-1.595039	-0.197071
C15	-2.957430	-2.417900	-0.005800
O15	-2.765337	-3.673532	0.367586
C16	0.023830	1.548085	-0.332211
C17	1.476331	1.067454	-0.122251
C18	1.417536	-0.459007	0.280407
C19	2.781694	-1.167903	-0.114220
C20	-0.202076	2.835896	0.609680
O20	-1.586609	3.136011	0.915965
N21	0.462156	3.871380	-0.189410
C22	0.073463	3.629009	-1.518808
N22	-0.142030	4.550880	-2.401389
N23	-0.031625	2.273682	-1.654568
N24	3.767756	-1.070334	0.981465
C25	4.268856	-2.196097	1.596671
O25	3.913764	-3.334219	1.257292
C26	5.276748	-2.068179	2.713066
C27	5.794256	-0.848844	3.228235
C28	6.691558	-1.192090	4.244494
C29	6.694675	-2.623439	4.319526
N30	5.839099	-3.090318	3.390226
Cl17	2.472443	2.026108	0.934810
Br2	-8.361897	-2.358061	-0.323050
Br3	-7.069210	0.959667	-1.218473
Br28	7.700941	0.003184	5.308072
Br29	7.725115	-3.664734	5.518372
H1	-5.551045	-3.659027	0.211000
H6	-3.449835	0.716873	0.178364
H7	-3.771808	2.430457	-1.449313
H81	-2.939299	2.640893	-3.930821
H82	-1.829580	1.425517	-4.533246
H9	-1.467994	-0.697509	-3.025454
H11	-0.994275	0.145341	0.778433
H12	0.489514	-0.801083	-1.649506
H131	-0.566412	-2.927831	-0.998940
H132	-0.361982	-2.546967	0.710189
H17	1.975379	1.054659	-1.091213
H18	1.233260	-0.594249	1.346170
H191	2.597973	-2.171165	-0.498685
H192	3.230208	-0.556021	-0.896866
H20	0.373260	2.718050	1.527939
H20X	-1.955348	2.510658	1.573326
H21	1.071333	4.613241	0.105202
H221	-0.024822	5.536837	-2.143301
H222	-0.424573	4.326457	-3.342484
H23	-0.067073	1.770859	-2.553648
H24	4.087769	-0.121649	1.289325
H27	5.545472	0.160486	2.900425
H30	5.638043	-4.098942	3.216470

3,7-epi-Massadine chloride (3)



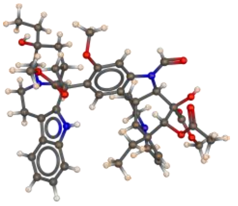
3,7-epi-Massadine chloride (3)			
C1	-0.288321	-0.446101	0.084231
C2	-1.819544	-0.586497	-0.197564
C3	-2.270217	-0.024611	-1.602974
O3	-1.566062	1.057332	-2.087571
N4	-2.280952	-1.156687	-2.634298
C5	-3.447196	-1.927778	-2.424102
N5	-3.667261	-3.259126	-2.830780
N6	-4.374152	-1.120815	-1.723730
C7	-3.804305	0.262466	-1.561674
O8	-4.317745	0.981280	-0.529668
C9	-3.939253	0.487428	0.833629
N10	-4.087030	1.788590	1.716981
C11	-2.983745	2.582060	1.393628
N11	-2.825251	3.931376	1.743880
N12	-2.062277	1.823131	0.666185
C13	-2.473969	0.293914	0.901396
C14	-1.634136	-0.086251	2.121581
C15	-0.172525	-0.045106	1.598072
Cl14	-1.942049	-1.760608	2.717294
H1	0.062163	0.451819	-0.424688
H2	-2.187049	-1.606934	-0.089180
H3X	-0.949981	0.872402	-2.817320
H4	-1.600715	-1.245376	-3.310749
H51	-2.927425	-3.774689	-3.342158
H52	-4.573508	-3.717473	-2.615175
H6	-5.274789	-1.415948	-1.383207
H7	-4.000849	0.733298	-2.524891
H9	-4.807476	-0.117872	1.094208
H10	-4.817797	1.924686	2.326243
H111	-3.566580	4.412341	2.287071
H112	-1.966711	4.439193	1.456637
H12	-1.328216	2.079558	0.137144
H14	-1.802662	0.580448	2.967283
H15	0.444998	-0.833550	2.028330
C1A	0.612632	-1.637362	-0.304263
N2A	1.834741	-1.723280	0.620476
C3A	2.459528	-2.871791	0.746124
O3A	2.059735	-3.949978	0.095804
C4A	3.670567	-3.013757	1.645627
N5A	4.235995	-1.979983	2.411684
C6A	5.322003	-2.470085	3.104507
C7A	5.469716	-3.828085	2.792709
C8A	4.436684	-4.170151	1.879527
Br6A	6.344012	-1.382732	4.243712
Br7A	6.810410	-4.969312	3.479735
H1A1	1.061330	-1.459378	-1.281551
H1A2	0.123469	-2.608733	-0.231760
H2A	2.115682	-0.889226	1.102327
H5A	3.926197	-1.015722	2.473439
H8A	4.254449	-5.146550	1.430599
C1B	0.577512	1.292552	1.808972
N2B	1.002545	1.890009	0.508464
C3B	2.155464	1.478715	-0.163229
O3B	2.878351	0.577192	0.256285
C4B	2.518953	2.177441	-1.459668
N5B	1.782131	3.219417	-2.050214
C6B	2.404181	3.610105	-3.215829
C7B	3.550994	2.823927	-3.391562
C8B	3.622922	1.926893	-2.292097
Br6B	1.715132	4.984951	-4.293299
Br7B	4.758215	2.959022	-4.838512
H1B1	0.087610	2.063470	2.403767
H1B2	1.529803	1.034374	2.272207
H2B	0.458178	2.670537	0.125401
H5B	0.927223	3.642594	-1.706311
H8B	4.389580	1.173391	-2.111625

Tubocurarine (4)



Tubocurarine (4)			
C1	0.837179	-1.444167	-3.070455
N2	1.758805	-2.058683	-4.120049
C3	1.316272	-3.496275	-4.448324
C4	-0.056078	-3.503147	-5.119821
C5	-1.037529	-2.506479	-4.521688
C6	-2.396002	-2.537288	-4.932564
C7	-3.314727	-1.648866	-4.414390
C8	-2.909009	-0.679739	-3.460850
C9	-1.551817	-0.657466	-3.054145
C10	-0.634512	-1.563625	-3.594658
C11	1.789163	-1.199324	-5.385218
C12	3.205019	-2.129448	-3.582266
O13	-4.647910	-1.563265	-4.716474
C14	-5.048278	-1.753237	-6.106469
O15	-3.767929	0.213435	-2.919882
O16	-1.131790	0.261223	-2.145839
C17	-1.465266	0.304364	-0.798557
C18	-1.396084	1.565913	-0.223905
C19	-1.854598	-0.791078	-0.032300
C20	-1.732947	1.737230	1.124277
C21	-2.169688	-0.615418	1.320486
C22	-2.131847	0.649963	1.903575
C23	-2.495463	0.878020	3.363280
C24	-1.127312	0.707103	4.256148
N25	-1.536541	1.006531	5.678419
C26	-1.775832	2.465165	5.953456
C27	-0.634505	3.333286	5.606217
C28	0.156735	2.901386	4.348941
C29	1.160619	3.744340	3.851540
C30	1.904069	3.368732	2.733458
C31	1.668179	2.130693	2.132368
C32	0.679226	1.294193	2.622287
C33	-0.066826	1.675216	3.762030
C34	-0.626579	0.378698	6.710564
O35	2.916711	4.116440	2.172374
C36	3.364976	5.288442	2.921671
O37	2.460222	1.787312	1.009649
C38	2.575541	0.422185	0.689367
C39	1.757453	-0.126688	-0.267594
C40	3.521893	-0.353759	1.352731
O41	4.299965	0.288517	2.281963
C42	3.647066	-1.693263	1.026802
C43	2.806270	-2.279362	0.062400
C44	1.866777	-1.481761	-0.619175
C45	0.944252	-2.089617	-1.692943
H1	1.072131	-0.389355	-2.928083
H3A	2.060735	-3.876812	-5.147656
H3B	1.291659	-4.101384	-3.542047
H4A	0.096705	-3.226337	-6.162958
H4B	-0.481669	-4.504270	-5.051077
H6	-2.718931	-3.278785	-5.663316
H11A	1.772239	-1.881320	-6.235333
H11B	0.903559	-0.564339	-5.360731
H11C	2.707036	-0.612183	-5.355648
H12A	3.367407	-1.240012	-2.973469
H12B	3.279577	-3.040684	-2.988811
H12C	3.875615	-2.156450	-4.441144
H14A	-4.340058	-2.444371	-6.563479
H14B	-6.056990	-2.166260	-6.103275
H14C	-5.023304	-0.778718	-6.594106
H15	-4.177942	-0.152566	-2.197046
H18	-1.112618	2.408303	-0.854878
H19	-1.912536	-1.781246	-0.484308
H20	-1.696035	2.747084	1.532851
H21	-2.502355	-1.489155	1.880857
H23A	-2.826422	1.901637	3.538704
H23B	-3.212795	0.137039	3.716099
H24	-0.805268	-0.316445	4.064475
H25	-2.425335	0.499823	5.842692
H26A	-2.051635	2.556734	7.004002
H26B	-2.627108	2.830932	5.379310
H27A	-0.905504	4.389056	5.603180
H27B	0.113639	3.207688	6.388908
H29	1.342714	4.708108	4.327031
H32	0.507623	0.314627	2.176076
H34A	-0.416830	-0.643113	6.394324
H34B	0.282714	0.978498	6.749611
H34C	-1.156291	0.399030	7.662978
H36A	2.488342	5.902242	3.128704
H36B	3.826934	4.937318	3.844388
H36C	4.083525	5.825456	2.302476
H39	1.031002	0.485885	-0.801564
H41	5.026724	0.646153	1.870449
H42	4.375278	-2.324167	1.536475
H43	2.931328	-3.329093	-0.203163
H45A	-0.033557	-1.848175	-1.276175
H45B	0.978477	-3.178479	-1.729106

Vincristine (5)



Vincristine (5)			
N1	2.194340	-1.701936	1.341816
C2	1.082000	-2.523979	1.231127
C3	1.481953	-3.651177	0.466598
C4	2.872912	-3.438820	0.146227
C5	3.835553	-4.244180	-0.580964
C6	5.127633	-3.760030	-0.705905
C7	5.529306	-2.505055	-0.110232
C8	4.632041	-1.723246	0.588153
C9	-0.170682	-2.029077	1.945786
C10	-1.531905	-2.799599	1.674680
C11	0.959510	-4.981028	-0.076293
C12	-0.519399	-5.409219	-0.216700
N13	-1.403833	-4.559435	-1.084559
C14	-1.404892	-3.090981	-0.962120
C15	-2.194240	-2.585643	0.252430
C16	-3.634746	-3.162515	0.174623
C17	-3.767259	-4.676243	-0.107824
C18	-2.775342	-5.084019	-1.241080
C19	0.163405	-2.206281	3.423726
O20	0.940727	-1.425448	3.984501
O21	-0.418735	-3.254075	4.119892
C22	0.030532	-3.360464	5.471323
O23	-3.511470	-5.426975	1.085996
C24	-5.240332	-4.920483	-0.552980
C25	-5.691343	-6.387782	-0.716796
C26	-0.607303	-0.601355	1.632666
C27	-0.310203	-0.019774	0.388030
C28	-0.688595	1.317252	0.118234
C29	-1.429781	2.039872	1.043525
C30	-1.822768	1.463494	2.275306
C31	-1.381280	0.165385	2.576944
O32	-1.751112	-0.365965	3.835638
C33	-3.136128	-0.243432	4.163698
N34	-1.711799	3.306750	0.520883
C35	-2.458350	4.165478	1.177588
O36	-2.799815	5.299725	0.620787
C37	-1.129943	3.517052	-0.831607
C38	-0.436427	2.143154	-1.135040
C39	0.989576	2.224915	-1.662639
C40	1.992485	3.184792	-0.919069
C41	1.192452	4.298682	-0.143018
C42	-0.089531	4.717494	-0.880469
C43	-1.174105	1.414660	-2.337134
C44	-0.421370	1.867703	-3.593447
N45	0.752897	2.592341	-3.066724
C46	1.915730	2.780883	-3.924733
C47	2.933650	3.695187	-3.244088
C48	2.941271	3.858674	-1.903448
O49	-0.653949	5.864257	-0.272854
C50	0.256998	5.130175	-2.301361
O51	-0.510059	4.793682	-3.207243
O52	1.408449	5.865682	-2.550551
C53	1.530481	6.235772	-3.925487
O54	1.997309	5.476754	0.042285
C55	1.708340	6.300867	1.123328
O56	0.781075	6.153898	1.917988
C57	2.629472	7.492376	1.335611
C58	2.849063	2.449937	0.136748
C59	3.994167	1.538391	-0.387270
C60	3.271410	-2.215504	0.712112
H1	2.188287	-0.926053	1.809466
H5	3.535575	-5.196797	-1.017579
H6	5.862722	-4.367563	-1.233776
H7	6.563480	-2.176940	-0.214752
H8	4.920230	-0.783652	1.059544
H10A	-1.357719	-3.866417	1.814889
H10B	-2.249979	-2.376589	2.377198
H11A	1.337356	-5.717415	0.632979
H11B	1.414906	-5.159985	-1.050300
H12A	-0.978572	-5.316531	0.767510
H12B	-0.601900	-6.434519	-0.577327
H14A	-1.833922	-2.698185	-1.883936
H14B	-0.370079	-2.759110	-0.877722
H15	-2.213815	-1.496720	0.208121
H16A	-4.141895	-2.923183	1.109300
H16B	-4.130896	-2.638039	-0.641992
H18A	-3.143820	-4.695162	-2.190350
H18B	-2.738011	-6.172450	-1.286056
H22A	-0.704636	-2.862105	6.103198
H22B	0.107006	-4.419946	5.715762
H22C	1.001891	-2.869787	5.532943
H23	-3.660093	-4.904134	1.812753
H24A	-5.896168	-4.429933	0.166283
H24B	-5.366507	-4.420067	-1.513065
H25A	-5.425270	-6.753270	-1.708624
H25B	-5.201187	-7.012696	0.029749
H25C	-6.770820	-6.464760	-0.586783
H27	0.310642	-0.545944	-0.337089
H30	-2.361343	2.052541	3.017640
H33A	-3.704612	-0.322276	3.237032
H33B	-3.382784	-1.053274	4.850297
H33C	-3.275552	0.730771	4.632301
H35	-2.839634	3.973298	2.180479
H37	-1.823164	3.839335	-1.608573
H39	1.603744	1.339281	-1.499696
H41	0.975935	3.819982	0.812004
H43A	-1.054530	0.344659	-2.167132
H43B	-2.220516	1.719672	-2.346750
H44A	-0.030115	1.041595	-4.187219
H44B	-1.054010	2.507849	-4.208329
H46A	1.555438	3.260734	-4.834696
H46B	2.397125	1.831851	-4.160734
H47	3.656416	4.230736	-3.859635
H48	3.693861	4.526805	-1.484748
H49	-1.339472	6.186666	-0.773024
H53A	1.354548	5.340442	-4.521751
H53B	0.781078	7.000398	-4.130041
H53C	2.539281	6.620409	-4.075414
H57A	2.621255	7.779253	2.387150
H57B	3.644729	7.226099	1.041588
H57C	2.287540	8.331447	0.729688
H58A	3.297920	3.191164	0.797966
H58B	2.191263	1.826393	0.742217
H59A	4.798384	2.157075	-0.785473
H59B	4.377150	0.927940	0.430516
H59C	3.610737	0.890937	-1.175867