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Stereochemical analysis of natural products: alkaloids from the root bark of *Strychnos panganensis*

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Geographical description of the substances studied

The name of this species has been given because the first specimen has been discovered by Franz Stuhlmann, German naturalist and African explorer in the region of River Pangani that flows from the slopes of Mount Kilimanjaro till the historical town of Pangani that owes also its name to the river. The species was finally collected in three countries of East Africa (Tanzania, Kenya and Mozambique) where all the specimens are at least partly hairy while the rare specimens later discovered at the northernmost point of Madagascar are entirely glabrous.[S1] This point of taxonomy remains to be examined.

The ethnobotanical data are very rare about this species. Indeed, only two annotations from herbaria sheets collected in Kilifi District (Kenya) are found in the literature. The first one mentions the edibility of the fruits (small yellow subglobose berries) and the second one records the internal use of an undefined part of the plant against chest complaints.[S2]

Computational details

Conformational search and geometry optimization

The initial conformational search of panganensine alkaloids **1-4** was performed using the OPLS3 force field software in the liquid phase of chloroform using the MacroModel program implemented in Schrödinger Maestro 11.5 package[S3]. In the course of this search, as many as 10^5 steps were taken to find the most probable conformers. After that, the unique conformations of each of alkaloids were identified and subjected to a further geometry optimization with GAUSSIAN 09 [S4] at the M06-2X/pecG-2 level [S5-S7]. The solvent effect of chloroform was accounted for within the Integral Equation Formalism Polarizable Continuum Model (IEF-PCM).[S8,S9] All considered optimized structures of **1-4** were found to be the true minima on the potential energy surface, as was confirmed by the absence of imaginary frequencies at that computational level.

Calculation of chemical shifts

All calculations of ^{1}H and ^{13}C NMR isotropic magnetic shielding constants (the latter being converted into chemical shifts) were carried out at the GIAO-DFT level in the liquid phase of chloroform by implying the GAUSSIAN 09 code. In these calculations, we employed the one-parameter hybrid functional PBE0 [S10], which was used in combination with Rusakov′s basis set pecS-2 [S11,S12]. On the other hand, for DP4+ calculations we used the one-parameter hybrid functional mPW1PW91 (which is based on the Perdew-Wang exchange, as modified by Adamo and Barone combined with PW91 correlation [S13]). The latter was employed in combination with Pople's triple-zeta basis set 6-311G(*d*,*p*). [S14] Calculated proton and carbon isotropic magnetic shielding constants were then converted into the ^{1}H and ^{13}C NMR chemical shifts scale, as recommended by IUPAC. [S15]

To take into account the systematic errors of calculated chemical shifts, we have established correlations between their isotropic magnetic shielding constants (y) and experimental chemical shifts (x). Resulting linear regressions were further used to define the equations of the $y = ax + b$ type. The slope a and intercept b were used then for recalculating unscaled shielding constants (σ_{calc}) into their scaled values of chemical shifts (δ_s) as $\delta_s = (\sigma_{calc} - b)/a$.

Topological analysis

The wave functions obtained as a result of geometry optimization (M06-2X/pecG-2) were used for the further calculations to carry out the topological analysis of the real space functions. Analysis of the electron density using the obtained wave functions was performed with the AIMAll 19 program, [S16] the latter used to locate and visualize the (3,-1) bond critical points in the space of that descriptor.

Estimation of probability distribution of conformers

To analyze the distribution of conformers, we used the DP4+ approach, which was developed and introduced into practice by Sarotti. [S17,S18] The DP4+ formalism involves inclusion of the unscaled NMR chemical shifts in the probability calculation in combination with the implementation of the scaled NMR chemical shifts:

$$P_i = \frac{\prod_{k=1}^{N}\left[1 - T_s^{\nu}\left(\frac{e_{s,k}^{i}}{\sigma_s}\right)\right]\left[1 - T_{u-spx}^{\nu}\left(\frac{e_{u,k}^{i} - \mu_{u-spx}}{\sigma_{u-spx}}\right)\right]}{\sum_{j=1}^{m}\prod_{k=1}^{N}\left[1 - T_s^{\nu}\left(\frac{e_{s,k}^{i}}{\sigma_s}\right)\right]\left[1 - T_{u-spx}^{\nu}\left(\frac{e_{u,k}^{i} - \mu_{u-spx}}{\sigma_{u-spx}}\right)\right]}$$

where T_s^{ν}, and $T_{u\text{-}spx}^{\nu}$ are the standard cumulative *t*-distribution function with ν degrees of freedom centered on average calculation error μ and variance σ, corresponding to the scaled and unscaled NMR shielding constants taking into account type of hybridization of carbons. The scaled and unscaled deviations (errors) e_s, e_u for nucleus *k* can be evaluated as $e_{s,u} = \delta_{s,u} - \delta_{exp}$.

Thus, the prevailing conformer of each of the investigated alkaloids **1**-**4** was established and verified by applying the DP4+ analysis of the probability of each of the low-level energy candidate conformers.

Mean Absolute Errors (MAE) were evaluated as

$$MAE = \frac{\sum_{i=1}^{n}|e_i|}{n}$$

where e_i is the calculation error for each of *n* nuclei.

Corrected Mean Absolute Errors (CMAE) were calculated as

$$CMAE = \frac{\sum_{i=1}^{n}\left|\delta_{exp} - \left(\frac{\sigma_{calc} - b}{a}\right)\right|}{n}$$

where σ_{calc} are the unscaled values of NMR shielding constants for each of n nuclei, a and b are the slope and intercept of the linear regression $\sigma_{calc} = a\delta_{exp} + b$.

The Root Mean Square Deviations (RMSD) were evaluated as

$$RMSD = \sqrt{\frac{\sum_{i=1}^{n}(\delta_{exp} - \delta_{calc})^2}{n}}$$

while Pearson correlation coefficients r were calculated as

$$\boldsymbol{r}(\delta_{exp}, \delta_{calc}) = \frac{\sum_{i=1}^{n}\left((\delta_{exp} - \frac{\sum_{i=1}^{n}\delta_{exp}}{n})(\delta_{calc} - \frac{\sum_{i=1}^{n}\delta_{calc}}{n})\right)}{\sqrt{\sum_{i=1}^{n}(\delta_{exp} - \frac{\sum_{i=1}^{n}\delta_{exp}}{n})^2 \sum_{i=1}^{n}(\delta_{calc} - \frac{\sum_{i=1}^{n}\delta_{calc}}{n})^2}}$$

where δ_{exp} and δ_{calc} are the experimental and scaled NMR chemical shifts of each of the n nuclei, respectively.

Normalized values of considered descriptors (D) were evaluated as N(D) = (D) / Range (D) · 100%.

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Table S1. Calculated ^{1}H and ^{13}C NMR shielding constants and corresponding chemical shifts of main conformers of **1**-**4**, ppm**.**

Panganensine R (**1**)									
Nuclei	^{1}H NMR								
	Shielding constants				Chemical shifts				
	1a	**1b**	**1c**	**1d**	**1a**	**1b**	**1c**	**1d**	**Exp**
2	27.69	27.78	27.65	28.62	3.83	3.75	3.87	2.99	2.96
3	27.77	27.78	27.81	27.81	3.76	3.75	3.73	3.72	3.60
5a	28.08	28.05	28.01	28.10	3.48	3.50	3.54	3.46	3.50
5b	28.26	28.25	28.24	28.37	3.31	3.32	3.33	3.22	3.25
6a	28.77	28.78	28.82	28.97	2.85	2.84	2.81	2.67	2.46
6b	29.98	29.97	29.95	29.98	1.75	1.76	1.78	1.74	ND
9	24.04	24.02	24.04	24.03	7.16	7.17	7.16	7.16	7.05
10	24.44	24.43	24.43	24.43	6.80	6.81	6.81	6.80	6.75
11	24.08	24.08	24.08	24.09	7.12	7.12	7.12	7.11	7.05
12	24.60	24.60	24.58	24.61	6.65	6.65	6.67	6.64	6.60
14a	29.54	29.53	29.58	29.45	2.15	2.16	2.11	2.23	2.10
14b	29.62	29.56	29.58	29.78	2.07	2.13	2.11	1.93	1.85
15	28.96	28.99	29.33	28.94	2.68	2.65	2.34	2.70	2.80
16	30.19	30.14	30.08	29.82	1.56	1.60	1.66	1.89	1.75
17a	27.60	27.63	27.48	28.00	3.92	3.88	4.03	3.55	3.55
17b	27.86	27.93	27.71	27.90	3.67	3.62	3.82	3.64	ND
18	26.07	25.35	25.93	24.97	5.31	5.96	5.44	6.31	5.35
19	25.13	24.14	25.27	24.78	6.17	7.06	6.03	6.48	6.20
21	25.03	24.98	24.61	24.96	6.25	6.30	6.64	6.32	6.15
2'	27.81	27.87	27.78	27.79	3.73	3.67	3.75	3.75	3.80
3'	28.09	27.97	28.08	28.10	3.47	3.57	3.48	3.46	4.05

5'a	28.48	28.77	28.32	28.49	3.11	2.85	3.26	3.10	3.40
5'b	28.60	28.47	28.65	28.47	3.00	3.12	2.96	3.12	3.30
6'a	29.91	29.97	29.88	29.81	1.81	1.76	1.84	1.90	1.90
6'b	28.91	28.96	28.90	28.87	2.72	2.68	2.73	2.76	2.57
9'	24.06	24.05	24.08	24.06	7.14	7.15	7.12	7.14	7.10
10'	24.45	24.44	24.46	24.43	6.79	6.80	6.77	6.80	6.80
11'	24.11	24.12	24.11	24.10	7.09	7.09	7.09	7.10	7.10
12'	24.62	24.62	24.63	24.61	6.63	6.63	6.62	6.63	6.65
14'a	29.62	29.60	29.61	29.48	2.07	2.09	2.09	2.20	2.14
14'b	29.91	29.89	29.94	29.91	1.81	1.83	1.79	1.81	ND
15'	29.92	29.91	29.93	29.86	1.80	1.81	1.79	1.86	2.12
16'	30.37	30.38	30.39	30.38	1.39	1.39	1.37	1.39	1.37
17'a	27.66	27.67	27.66	27.67	3.86	3.85	3.86	3.85	3.85
17'b	28.01	27.99	28.01	28.02	3.54	3.56	3.54	3.53	3.55
18'a	30.53	30.13	30.51	30.50	1.25	1.61	1.27	1.28	1.25
19'	28.08	28.07	28.09	28.14	3.48	3.48	3.47	3.42	3.95
20'	30.06	30.14	30.13	29.69	1.67	1.60	1.62	2.02	1.54
21'	28.65	28.32	28.62	28.48	2.96	3.26	2.99	3.11	3.15
				^{13}C NMR					
2	118.1	118.1	120.6	112.5	61.9	61.9	59.6	67.2	66.1
3	122.3	122.4	122.7	121.8	58.0	57.8	57.5	58.4	58.1
5	131.4	131.7	131.9	131.3	49.4	49.1	48.9	49.4	50.3
6	142.6	143.2	143.3	141.1	38.9	38.3	38.2	40.3	40.7
7	123.7	123.4	122.9	123.5	56.6	56.9	57.4	56.8	55.4
8	42.5	42.7	43.5	42.1	133.0	132.8	132.0	133.3	131.4
9	53.6	53.4	53.2	53.6	122.5	122.7	122.9	122.5	121.7
10	59.1	58.9	58.6	58.6	117.4	117.6	117.8	117.8	118.8
11	47.6	47.6	47.4	47.7	128.2	128.2	128.3	128.1	127.9
12	68.3	68.2	67.9	68.1	108.7	108.8	109.0	108.9	110.0

13	22.4	22.4	22.0	22.1	151.9	151.8	152.2	152.1	150.3
14	153.6	153.2	154.3	156.2	28.5	28.9	27.8	26.1	27.0
15	151.2	150.1	145.3	152.0	30.8	31.8	36.3	30.0	25.5
16	133.6	134.1	133.9	132.0	47.3	46.9	47.0	48.8	48.9
17	118.3	117.9	116.0	117.8	61.7	62.0	63.9	62.2	63.8
18	48.3	49.6	43.0	42.9	127.5	126.3	132.4	132.6	ND
19	39.2	40.8	44.2	32.4	136.0	134.6	131.3	142.5	139.3
20	63.2	63.1	65.6	61.4	113.5	113.6	111.2	115.2	ND
21	31.3	30.7	38.4	42.0	143.5	144.1	136.8	133.5	141.4
2'	112.0	112.0	111.5	111.4	67.7	67.6	68.1	68.2	67.3
3'	120.6	120.2	120.2	119.6	59.5	59.9	59.9	60.5	60.2
5'	130.8	127.4	130.8	128.3	49.9	53.2	50.0	52.3	50.5
6'	139.0	139.0	138.2	138.8	42.3	42.2	43.0	42.4	41.5
7'	124.4	124.4	125.0	125.3	55.9	55.9	55.4	55.2	53.5
8'	39.9	39.8	39.6	40.4	135.4	135.5	135.7	134.9	132.4
9'	53.5	53.6	53.6	53.5	122.6	122.5	122.5	122.6	121.7
10'	58.6	58.6	58.8	58.5	117.8	117.8	117.6	117.9	119.5
11'	48.1	48.1	48.1	47.8	127.7	127.7	127.7	128.0	128.1
12'	68.4	68.4	68.6	68.4	108.6	108.6	108.4	108.6	110.0
13'	22.8	23.0	22.9	23.1	151.4	151.3	151.4	151.2	149.3
14'	154.5	154.6	154.5	155.0	27.6	27.6	27.7	27.2	26.6
15'	149.1	148.5	148.9	149.6	32.8	33.3	32.9	32.3	31.8
16'	139.4	139.1	139.3	139.1	41.9	42.1	41.9	42.2	42.2
17'	109.6	109.5	109.6	109.6	69.9	70.0	69.9	69.9	71.7
18'	161.3	162.2	160.5	161.8	21.3	20.5	22.1	20.8	21.5
19'	101.9	101.9	101.9	103.1	77.1	77.1	77.1	76.0	78.5
20'	137.6	133.5	138.2	135.3	43.6	47.4	43.0	45.7	42.7
21'	118.4	120.5	118.8	124.1	61.6	59.7	61.2	56.3	63.4

Panganensine S (**2**)									
^{1}H NMR									
	Shielding constants				Chemical shifts				
	2a	**2b**	**2c**	**2d**	**2a**	**2b**	**2c**	**2d**	**Exp**
2	27.75	28.77	27.69	28.17	3.7	2.8	3.8	3.3	2.95
3	27.75	27.76	27.80	27.81	3.7	3.7	3.7	3.7	3.70
5a	28.26	28.37	28.32	28.31	3.3	3.2	3.2	3.2	3.20
5b	28.05	28.08	28.09	28.11	3.4	3.4	3.4	3.4	3.45
6a	29.96	29.97	29.99	30.02	1.7	1.7	1.7	1.6	1.70
6b	28.78	28.95	28.83	28.85	2.8	2.6	2.7	2.7	2.45
9	24.04	24.04	24.04	24.05	7.1	7.1	7.1	7.1	7.02
10	24.43	24.41	24.44	24.46	6.7	6.8	6.7	6.7	6.74
11	24.09	24.07	24.09	24.10	7.0	7.1	7.1	7.0	7.05
12	24.61	24.57	24.61	24.65	6.6	6.6	6.6	6.5	6.59
14a	29.51	29.43	29.48	29.45	2.1	2.2	2.1	2.2	2.10
14b	29.59	29.64	29.63	29.68	2.0	2.0	2.0	2.0	1.90
15	28.92	28.47	29.39	29.57	2.7	3.1	2.2	2.1	2.30
16	30.13	29.95	30.14	30.06	1.5	1.7	1.5	1.6	1.75
17a	27.68	28.11	27.82	27.85	3.8	3.4	3.7	3.6	3.55
17b	27.88	27.94	27.83	27.77	3.6	3.5	3.6	3.7	3.90
18	25.20	25.87	25.04	25.92	6.0	5.4	6.2	5.4	5.35
19	24.30	24.99	24.55	25.36	6.9	6.2	6.6	5.9	6.08
21	24.98	25.04	24.88	24.94	6.2	6.2	6.3	6.3	6.10
2'	27.72	27.73	27.74	27.73	3.7	3.7	3.7	3.7	3.75
3'	27.99	28.05	27.99	28.08	3.5	3.4	3.5	3.4	3.72
5'a	28.60	28.37	28.52	28.48	2.9	3.2	3.0	3.1	3.30
5'b	28.49	28.55	28.39	28.60	3.0	3.0	3.1	2.9	3.15
6'a	29.81	29.87	29.87	29.83	1.8	1.8	1.8	1.8	1.85

6'b	28.95	28.89	28.92	28.95	2.6	2.7	2.6	2.6	2.50
9'	24.03	24.08	24.05	24.07	7.1	7.1	7.1	7.1	7.02
10'	24.44	24.44	24.43	24.45	6.7	6.7	6.7	6.7	6.77
11'	24.11	24.09	24.12	24.11	7.0	7.1	7.0	7.0	7.05
12'	24.63	24.61	24.62	24.63	6.6	6.6	6.6	6.6	6.62
14'a	29.70	29.73	29.74	29.67	1.9	1.9	1.9	2.0	2.15
14'b	29.97	29.91	29.94	29.96	1.7	1.8	1.7	1.7	1.70
15'	29.62	29.62	29.61	29.60	2.0	2.0	2.0	2.0	1.80
16'	30.40	30.40	30.39	30.40	1.3	1.3	1.3	1.3	1.35
17'a	28.05	28.08	28.06	28.07	3.4	3.4	3.4	3.4	3.65
17'b	27.62	27.65	27.63	27.64	3.8	3.8	3.8	3.8	3.65
18'a	30.23	30.37	30.29	30.29	1.5	1.3	1.4	1.4	1.15
19'	27.35	27.69	27.3558	27.35	4.1	3.8	4.1	4.1	3.50
20'	30.35	30.29	30.3642	30.36	1.4	1.4	1.3	1.3	1.75
21'	28.33	28.75	28.3066	28.77	3.2	2.8	3.2	2.8	3.10
				^{13}C NMR					
2	118.5	115.5	118.1	107.6	61.7	64.5	62.1	72.0	66.2
3	122.3	122.2	122.4	122.6	58.2	58.2	58.0	57.9	58.0
5	131.5	131.3	131.6	131.4	49.5	49.7	49.4	49.6	50.1
6	142.9	142.0	142.4	141.7	38.9	39.7	39.3	39.9	40.6
7	124.0	123.2	123.7	122.8	56.6	57.3	56.8	57.7	55.4
8	42.8	42.7	42.4	41.8	132.7	132.8	133.1	133.7	131.2
9	53.4	53.5	53.5	53.7	122.7	122.7	122.7	122.5	121.6
10	59.0	58.5	59.0	59.3	117.5	118.0	117.5	117.3	118.8
11	47.6	47.6	47.7	47.7	128.2	128.2	128.1	128.2	127.9
12	68.3	67.9	68.3	68.4	108.8	109.2	108.8	108.7	110.1
13	22.4	21.9	22.2	22.3	151.9	152.3	152.1	151.9	150.3
14	153.5	156.3	153.9	154.7	28.8	26.2	28.5	27.8	29.6
15	151.3	156.5	142.9	147.8	30.9	26.1	38.8	34.2	25.6

16	134.1	132.2	134.2	131.2	47.0	48.9	47.0	49.8	48.9
17	118.1	118.5	117.9	106.2	62.1	61.7	62.2	73.3	63.5
18	52.8	47.4	45.8	40.8	123.4	128.4	129.9	134.6	ND
19	43.0	40.6	41.7	37.4	132.6	134.8	133.8	137.8	140.6
20	62.9	63.0	63.5	62.1	113.9	113.8	113.3	114.6	113.2
21	30.8	32.9	39.0	38.8	144.0	142.1	136.3	136.5	143.2
2'	111.0	112.6	112.0	111.5	68.8	67.2	67.8	68.3	66.9
3'	118.5	120.4	119.6	119.2	61.7	60.0	60.7	61.0	60.5
5'	127.7	129.8	128.1	129.5	53.0	51.1	52.7	51.4	50.4
6'	137.4	139.6	138.4	137.7	44.0	42.0	43.1	43.7	42.0
7'	125.2	125.0	124.7	125.7	55.4	55.6	55.9	55.0	52.7
8'	39.3	40.3	39.7	39.4	136.0	135.0	135.7	135.9	131.2
9'	53.6	53.5	53.6	53.5	122.6	122.7	122.6	122.7	122.3
10'	58.8	58.5	58.6	58.8	117.8	118.0	117.9	117.8	119.8
11'	48.1	47.8	48.0	48.1	127.8	128.0	127.8	127.8	128.6
12'	68.6	68.2	68.5	68.6	108.5	108.9	108.7	108.5	110.1
13'	23.2	22.8	23.0	23.0	151.1	151.5	151.3	151.4	149.1
14'	154.9	155.2	155.1	155.0	27.6	27.2	27.4	27.5	25.4
15'	156.9	157.6	157.1	157.0	25.6	25.0	25.5	25.5	23.3
16'	138.2	139.6	138.7	138.8	43.2	41.9	42.7	42.6	40.3
17'	118.6	119.1	119.0	118.7	61.6	61.2	61.3	61.6	62.4
18'	169.0	168.6	168.3	168.3	14.4	14.7	15.0	15.0	16.0
19'	109.8	109.4	110.1	110.6	69.8	70.2	69.6	69.1	69.5
20'	134.5	138.5	137.0	139.6	46.7	42.9	44.4	41.9	42.2
21'	119.9	114.9	119.6	116.0	60.4	65.1	60.6	64.1	67.0

Panganensine X (**3**)													
^{1}H NMR													
	Shielding constants						Chemical shifts						
	3a	**3b**	**3c**	**3d**	**3e**	**3f**	**3a**	**3b**	**3c**	**3d**	**3e**	**3f**	**Exp**
2	27.85	27.81	27.80	27.83	28.28	27.82	3.51	3.54	3.55	3.52	3.11	3.53	3.65
3	27.80	27.75	27.92	27.89	27.93	27.92	3.55	3.60	3.44	3.47	3.43	3.44	3.50
5a	28.34	28.34	28.63	28.71	28.40	28.63	3.06	3.06	2.80	2.73	3.00	2.80	3.17
5b	28.07	28.13	28.32	28.32	28.16	28.32	3.31	3.26	3.08	3.08	3.22	3.08	3.27
6a	29.98	29.96	30.14	30.04	30.16	30.14	1.58	1.59	1.43	1.52	1.41	1.43	1.94
6b	28.81	29.10	28.88	28.88	28.96	28.88	2.64	2.38	2.58	2.57	2.50	2.57	1.94
9	24.02	24.00	24.14	24.01	24.19	24.15	6.97	6.99	6.87	6.98	6.81	6.86	7.05
10	24.39	24.11	24.44	24.38	24.47	24.43	6.64	6.89	6.59	6.65	6.56	6.60	6.76
11	24.04	23.97	24.11	24.02	24.17	24.09	6.95	7.01	6.89	6.97	6.84	6.91	7.02
12	24.47	24.23	24.63	24.44	24.75	24.60	6.56	6.78	6.42	6.59	6.31	6.44	6.60
14a	29.92	29.85	29.86	29.78	29.96	29.83	1.64	1.69	1.68	1.75	1.60	1.72	1.98
14b	28.81	29.97	29.43	28.59	29.60	29.47	2.63	1.59	2.07	2.84	1.92	2.04	1.64
15	29.61	29.84	28.74	29.11	29.06	29.15	1.91	1.70	2.70	2.37	2.41	2.33	1.78
16	30.04	29.45	29.11	29.76	31.98	29.19	1.53	2.05	2.36	1.77	-0.24	2.30	1.71
17a	28.37	28.24	27.95	28.10	28.56	28.14	3.03	3.15	3.42	3.28	2.87	3.25	3.42
17b	27.72	28.71	28.38	27.67	29.07	28.39	3.63	2.73	3.03	3.67	2.41	3.02	3.23
18a	30.35	30.35	30.17	30.23	30.21	30.18	1.24	1.24	1.40	1.35	1.37	1.40	1.37
19	28.20	28.01	28.21	28.19	27.97	28.21	3.19	3.36	3.18	3.20	3.40	3.18	3.25
21	25.14	25.21	26.12	26.46	25.09	26.10	5.95	5.89	5.07	4.76	6.00	5.09	5.63
2'	27.41	27.39	27.33	27.36	27.32	27.33	3.90	3.92	3.98	3.95	3.99	3.98	3.45
3'	28.02	28.02	28.01	28.03	28.01	28.01	3.35	3.35	3.36	3.34	3.36	3.36	3.25
5'a	28.43	28.43	28.41	28.43	28.38	28.41	2.98	2.98	3.00	2.98	3.03	3.00	3.13
5'b	28.71	28.71	28.67	28.70	28.66	28.67	2.72	2.73	2.77	2.73	2.77	2.77	2.80
6'a	28.80	28.81	28.76	28.75	28.65	28.76	2.65	2.64	2.68	2.69	2.78	2.68	2.50

6'b	29.75	29.74	29.70	29.70	29.79	29.70	1.78	1.79	1.83	1.83	1.75	1.83	1.80
9'	24.03	24.16	24.07	24.27	24.05	24.07	6.96	6.84	6.93	6.74	6.95	6.93	6.92
11'	24.31	24.18	24.31	24.19	24.15	24.32	6.71	6.82	6.71	6.82	6.85	6.70	6.94
12'	24.77	24.70	24.70	24.62	24.71	24.70	6.29	6.36	6.35	6.43	6.35	6.36	6.59
14'	29.77	29.76	29.71	29.74	29.72	29.71	1.77	1.78	1.82	1.79	1.81	1.83	1.94
14'	29.87	29.83	29.76	29.85	29.82	29.76	1.68	1.71	1.78	1.69	1.72	1.77	1.71
15'	28.60	28.56	28.53	28.56	28.54	28.53	2.83	2.86	2.89	2.87	2.88	2.89	2.70
16'	30.21	30.12	30.07	30.15	30.14	30.07	1.37	1.45	1.50	1.43	1.43	1.50	1.79
17'	27.56	27.51	27.50	27.52	27.86	27.50	3.77	3.81	3.82	3.80	3.50	3.83	3.70
17'	27.89	27.86	27.83	27.86	27.52	27.83	3.47	3.49	3.53	3.50	3.80	3.53	3.53
18'	29.70	29.69	29.68	29.69	29.68	29.68	1.83	1.84	1.85	1.84	1.85	1.85	1.58
19'	25.58	25.58	25.57	25.57	25.56	25.56	5.56	5.56	5.57	5.57	5.58	5.57	5.50
21'	28.11	28.12	28.10	28.09	28.05	28.10	3.27	3.26	3.28	3.29	3.32	3.28	3.45
21'	28.18	28.22	28.16	28.18	28.19	28.17	3.20	3.17	3.22	3.21	3.20	3.22	3.00
						^{13}C NMR							
2	115.7	113.5	116.1	116.7	116.3	115.7	63.3	65.3	63.0	62.4	62.8	63.3	63.6
3	123.2	122.0	123.9	123.8	123.3	123.9	56.4	57.5	55.7	55.9	56.3	55.7	62.1
5	131.2	129.7	131.5	132.1	131.1	131.4	49.0	50.3	48.7	48.2	49.1	48.8	53.9
6	142.4	136.9	141.9	142.7	142.2	141.9	38.6	43.7	39.1	38.3	38.8	39.1	ND
7	124.3	121.4	124.3	124.9	124.4	124.3	55.3	58.1	55.4	54.8	55.2	55.4	54.4
8	42.3	31.3	41.3	42.7	41.6	41.7	131.2	141.4	132.1	130.9	131.9	131.8	137.2
9	52.8	54.5	54.8	52.7	54.8	54.9	121.5	119.9	119.6	121.5	119.6	119.5	121.5
10	57.9	52.9	58.5	57.9	58.2	58.4	116.8	121.4	116.3	116.8	116.5	116.3	119.5
11	47.0	47.8	47.9	46.9	47.9	47.6	126.9	126.1	126.0	126.9	126.0	126.3	127.5
12	68.2	60.4	69.1	68.1	68.6	68.9	107.3	114.4	106.4	107.3	106.9	106.6	109.5
13	22.8	23.6	22.1	22.5	22.2	22.1	149.2	148.5	149.9	149.5	149.8	149.9	150.1
14	158.1	160.9	161.7	157.4	161.7	162.0	24.2	21.5	20.7	24.8	20.8	20.5	23.6
15	147.1	147.6	152.6	145.3	156.8	152.1	34.3	33.8	29.2	36.0	25.3	29.7	29.2
16	136.9	134.6	135.4	135.0	135.4	133.8	43.7	45.9	45.1	45.5	45.1	46.6	45.3

17	115.5	114.7	119.6	116.0	119.8	119.0	63.5	64.2	59.7	63.0	59.6	60.2	64.0
18	162.0	161.7	162.0	164.1	165.9	162.0	20.5	20.8	20.5	18.5	16.9	20.5	20.1
19	137.7	137.9	134.4	134.8	136.1	134.4	42.9	42.8	46.1	45.7	44.5	46.1	43.8
20	53.9	54.5	52.8	50.6	54.0	53.9	120.5	119.9	121.5	123.6	120.4	120.4	127.0
21	39.9	40.2	36.5	36.9	40.3	36.2	133.4	133.2	136.5	136.2	133.0	136.8	131.1
2'	112.8	113.3	113.0	113.1	113.5	113.0	66.0	65.6	65.8	65.8	65.4	65.8	72.0
3'	117.1	117.3	116.9	117.1	117.2	116.9	62.1	61.9	62.2	62.1	61.9	62.2	61.9
5'	127.1	127.1	127.0	127.1	127.1	127.0	52.8	52.8	52.9	52.8	52.7	52.9	53.5
6'	137.7	137.8	137.9	137.5	136.3	137.8	42.9	42.9	42.8	43.1	44.2	42.9	42.9
7'	126.1	126.2	126.1	125.8	126.3	126.1	53.8	53.6	53.7	54.0	53.6	53.7	53.4
8'	38.8	40.0	39.7	40.0	38.5	39.6	134.4	133.4	133.6	133.3	134.7	133.7	133.6
9'	55.8	52.4	54.0	51.3	50.0	54.0	118.8	121.9	120.4	122.9	124.1	120.4	121.2
10'	36.5	36.5	39.0	39.7	38.4	39.4	136.5	136.6	134.2	133.6	134.8	133.9	136.1
11'	47.5	50.6	47.2	50.1	50.9	47.2	126.4	123.6	126.7	123.9	123.2	126.7	127.1
12'	69.7	68.2	69.3	69.0	71.5	69.3	105.9	107.2	106.2	106.5	104.2	106.2	109.8
13'	25.5	25.4	25.3	25.4	24.6	25.2	146.7	146.9	146.9	146.8	147.6	147.0	147.2
14'	152.5	152.8	152.3	152.7	152.7	152.3	29.3	29.0	29.4	29.1	29.1	29.5	28.3
15'	147.4	147.4	147.6	147.5	147.5	147.6	34.0	34.0	33.8	33.9	33.9	33.8	29.7
16'	131.0	130.9	131.0	131.3	131.3	131.0	49.2	49.3	49.2	48.9	48.9	49.2	48.3
17'	115.2	115.1	115.2	115.1	115.4	115.2	63.8	63.9	63.8	63.9	63.6	63.8	67.1
18'	170.6	170.6	170.6	170.5	170.6	170.6	12.6	12.6	12.6	12.6	12.6	12.6	12.8
19'	53.6	53.5	53.5	53.5	53.3	53.4	120.7	120.8	120.9	120.8	121.1	120.9	120.9
20'	28.5	28.6	28.7	28.7	29.0	28.7	143.9	143.8	143.8	143.8	143.5	143.8	135.1
21'	121.9	121.8	121.8	121.8	121.7	121.8	57.6	57.6	57.7	57.7	57.7	57.7	58.1

Panganensine Y (**4**)									
					^{1}H NMR				
	Shielding constants				Chemical shifts				
	4a	**4b**	**4c**	**4d**	**4a**	**4b**	**4c**	**4d**	**Exp**
2	28.30	28.32	27.78	27.73	3.0	3.0	3.5	3.6	3.71
3	27.83	27.94	27.85	27.87	3.5	3.4	3.5	3.5	3.27
5a	28.39	28.40	28.80	28.88	3.0	2.9	2.6	2.5	3.30
5b	28.21	28.13	28.33	28.35	3.1	3.2	3.0	3.0	3.30
6a	30.02	30.16	30.08	30.10	1.4	1.3	1.4	1.3	2.00
6b	29.19	28.95	28.95	28.96	2.2	2.4	2.4	2.4	2.00
9	24.04	24.19	24.01	24.01	7.1	6.9	7.1	7.1	7.01
10	24.14	24.48	24.38	24.38	7.0	6.7	6.8	6.8	6.70
11	24.03	24.16	24.02	24.01	7.1	7.0	7.1	7.1	6.95
12	24.37	24.74	24.43	24.43	6.8	6.4	6.7	6.7	6.56
14a	29.80	29.89	29.72	29.70	1.6	1.5	1.7	1.7	1.56
14b	29.99	29.63	28.58	28.54	1.4	1.8	2.8	2.8	1.90
15	29.78	29.20	29.06	29.11	1.6	2.2	2.3	2.3	1.63
16	31.70	31.87	29.78	29.65	-0.2	-0.3	1.6	1.8	1.83
17a	28.43	28.54	28.14	28.08	2.9	2.8	3.2	3.2	3.30
17b	28.80	29.04	27.58	27.53	2.6	2.3	3.7	3.8	3.47
18a	30.15	30.14	30.20	30.22	1.3	1.3	1.2	1.2	1.30
19	28.38	28.32	28.13	28.15	3.0	3.0	3.2	3.2	3.30
21	25.30	25.18	26.34	26.43	5.9	6.0	4.9	4.8	5.75
2'	27.40	27.31	27.34	27.35	3.9	4.0	3.9	3.9	3.42
3'	28.05	28.00	27.97	28.07	3.3	3.3	3.4	3.3	3.55
5'a	28.42	28.38	28.39	28.44	2.9	3.0	3.0	2.9	3.20
5'b	28.70	28.67	28.68	28.68	2.7	2.7	2.7	2.7	2.78
6'a	28.78	28.67	28.72	28.77	2.6	2.7	2.6	2.6	2.48

6'b	29.83	29.77	29.69	29.79	1.6	1.6	1.7	1.6	1.78
9'	24.23	24.00	23.96	24.33	6.9	7.1	7.2	6.8	6.82
11'	24.20	24.29	24.37	24.07	6.9	6.8	6.8	7.1	6.84
12'	24.63	24.77	24.66	24.70	6.5	6.4	6.5	6.5	6.49
14'a	29.98	29.72	29.74	29.69	1.4	1.7	1.7	1.7	1.94
14'b	29.34	29.82	29.85	29.83	2.1	1.6	1.6	1.6	1.68
15'	28.61	28.52	28.56	28.57	2.7	2.8	2.8	2.8	2.68
16'	29.58	30.11	30.15	30.13	1.8	1.3	1.3	1.3	1.76
17'a	27.60	27.51	27.85	27.54	3.7	3.8	3.5	3.8	3.50
17'b	27.90	27.86	27.52	27.84	3.4	3.5	3.8	3.5	3.63
18'a	29.74	29.68	29.68	29.72	1.7	1.7	1.7	1.7	1.60
19'	25.64	25.54	25.56	25.59	5.6	5.7	5.6	5.6	5.40
21'a	28.10	28.07	28.08	28.08	3.2	3.3	3.2	3.2	3.48
21'b	28.17	28.21	28.16	28.16	3.2	3.1	3.2	3.2	3.03
				^{13}C NMR					
2	113.6	116.3	116.0	114.5	65.7	63.1	63.4	64.8	63.7
3	122.0	123.4	123.1	122.9	57.9	56.5	56.9	57.1	61.8
5	129.9	131.1	131.5	130.7	50.5	49.4	49.0	49.7	53.5
6	136.5	142.3	142.6	141.8	44.4	39.0	38.7	39.5	40.6
7	122.4	124.6	124.3	124.4	57.5	55.5	55.7	55.7	54.5
8	31.0	41.7	42.2	41.8	142.5	132.5	132.0	132.4	136.9
9	54.8	54.8	52.8	53.0	120.4	120.3	122.1	122.0	121.5
10	52.9	58.2	57.9	58.0	122.1	117.1	117.5	117.4	119.4
11	48.0	47.9	47.0	47.0	126.6	126.8	127.6	127.6	127.5
12	60.6	68.6	68.2	68.2	114.9	107.5	107.8	107.8	109.7
13	24.3	22.3	22.9	22.9	148.7	150.6	149.9	150.0	150.0
14	160.4	161.7	158.0	158.6	22.2	21.0	24.4	23.8	23.1
15	144.7	151.4	146.3	145.8	36.8	30.5	35.3	35.8	28.4
16	136.4	136.0	136.5	136.6	44.5	44.8	44.4	44.3	45.1

17	116.1	119.8	115.1	115.2	63.3	59.9	64.3	64.2	64.7
18	164.8	166.2	165.6	165.4	18.1	16.8	17.3	17.5	20.7
19	135.1	136.0	138.6	138.4	45.7	44.8	42.4	42.6	42.2
20	53.2	54.4	48.0	47.7	121.8	120.7	126.6	126.9	126.2
21	43.2	42.0	36.8	35.6	131.1	132.2	137.1	138.2	130.7
2'	113.1	113.5	113.1	113.1	66.2	65.8	66.2	66.1	71.8
3'	117.6	116.8	117.5	117.0	62.0	62.7	62.0	62.5	61.8
5'	127.3	127.0	127.1	127.1	52.9	53.2	53.1	53.1	53.3
6'	139.7	136.3	138.0	138.5	41.4	44.6	43.0	42.6	42.1
7'	125.9	126.3	125.5	126.2	54.2	53.9	54.6	54.0	53.7
8'	39.9	38.0	41.2	39.0	134.2	136.0	132.9	135.0	133.0
9'	52.9	53.5	55.6	51.1	122.1	121.5	119.6	123.8	120.9
10'	37.8	37.3	39.3	38.5	136.1	136.6	134.7	135.5	137.1
11'	49.8	46.8	45.8	51.4	125.0	127.7	128.7	123.5	127.0
12'	68.0	71.5	68.4	71.0	108.1	104.8	107.6	105.3	109.8
13'	24.1	24.3	25.9	25.5	148.8	148.7	147.1	147.5	147.5
14'	153.9	152.8	152.9	152.4	28.2	29.3	29.2	29.6	27.9
15'	147.2	147.6	147.3	147.5	34.4	34.0	34.3	34.2	28.9
16'	133.7	131.0	131.2	131.4	47.0	49.5	49.3	49.1	48.2
17'	115.0	115.3	115.2	115.3	64.3	64.1	64.1	64.1	66.6
18'	170.7	170.6	170.5	170.6	12.6	12.7	12.8	12.7	12.7
19'	54.4	53.2	53.5	53.4	120.7	121.8	121.5	121.6	121.5
20'	27.7	29.0	28.5	28.8	145.5	144.3	144.7	144.5	134.3
21'	121.4	121.8	121.7	121.6	58.5	58.1	58.1	58.2	57.7

Table S2. Corrected mean absolute error (CMAE) and root mean square deviation (RMSD) of the main conformers of **1-4.**

Conformer	CMAE, ppm		RMSD, ppm	
	^{1}H	^{13}C	^{1}H	^{13}C
1a	0.16	1.50	0.24	1.85
2b	0.14	1.37	0.20	1.79
3b	0.17	2.21	0.21	3.09
4c	0.24	2.08	0.33	3.16
Average	0.18	1.79	0.25	2.47

Figure S1. DP4+ probability distribution (%) of the main energy low-level conformers of **1-4**, obtained by correlating experimental *versus* calculated at the mPW1PW91/6-311G(*d*,*p*) level ^{1}H and ^{13}C NMR data.

Panganensine R (**1**)

	a	*b*	*c*	*d*
*s*DP4+ (*^{1}H data*)	15.0	0.0	0.3	84.7
*s*DP4+ (*^{13}C data*)	98.9	0.0	0.0	1.1
***s*DP4+ (*all data*)**	94.3	0.0	0.0	5.7
*u*DP4+ (*^{1}H data*)	99.8	0.0	0.2	0.0
*u*DP4+ (*^{13}C data*)	86.1	0.3	13.6	0.0
***u*DP4+ (*all data*)**	100.0	0.0	0.0	0.0
DP4+ (*^{1}H data*)	100.0	0.0	0.0	0.0
DP4+ (*^{13}C data*)	100.0	0.0	0.0	0.0
DP4+ (*all data*)	100.0	0.0	0.0	0.0

Panganensine S (**2**)

	a	*b*	*c*	*d*
*s*DP4+ (*^{1}H data*)	0.0	97.8	0.0	2.2
*s*DP4+ (*^{13}C data*)	0.0	100.0	0.0	0.0
***s*DP4+ (*all data*)**	0.0	100.0	0.0	0.0
*u*DP4+ (*^{1}H data*)	96.1	3.9	0.0	0.0
*u*DP4+ (*^{13}C data*)	7.1	92.9	0.0	0.0
***u*DP4+ (*all data*)**	65.5	34.5	0.0	0.0
DP4+ (*^{1}H data*)	0.0	100.0	0.0	0.0
DP4+ (*^{13}C data*)	0.0	100.0	0.0	0.0
DP4+ (*all data*)	0.0	100.0	0.0	0.0

Panganensine X (**3**)

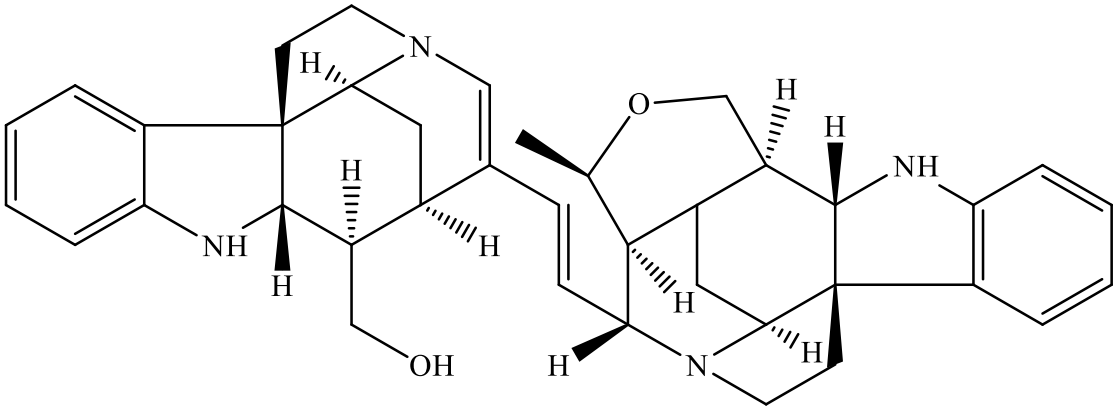
	a	*b*	*c*	*d*	*e*	*f*
*s*DP4+ (*^{1}H data*)	0.1	99.9	0.0	0.0	0.0	0.0
*s*DP4+ (*^{13}C data*)	95.9	2.4	0.3	1.4	0.0	0.0
***s*DP4+ (*all data*)**	2.5	97.5	0.0	0.0	0.0	0.0
*u*DP4+ (*^{1}H data*)	0.0	100.0	0.0	0.0	0.0	0.0
*u*DP4+ (*^{13}C data*)	0.3	99.7	0.0	0.0	0.0	0.0
***u*DP4+ (*all data*)**	0.0	100.0	0.0	0.0	0.0	0.0
DP4+ (*^{1}H data*)	0.0	100.0	0.0	0.0	0.0	0.0
DP4+ (*^{13}C data*)	11.4	88.6	0.0	0.0	0.0	0.0
DP4+ (*all data*)	0.0	100.0	0.0	0.0	0.0	0.0

Panganensine Y (**4**)

	a	*b*	*c*	*d*
*s*DP4+ (*^{1}H data*)	5.3	0.2	91.1	3.4
*s*DP4+ (*^{13}C data*)	0.0	0.0	96.9	3.1
***s*DP4+ (*all data*)**	0.0	0.0	99.9	0.1
*u*DP4+ (*^{1}H data*)	13.8	0.0	82.8	3.5
*u*DP4+ (*^{13}C data*)	71.8	0.8	15.0	12.4
***u*DP4+ (*all data*)**	43.4	0.0	54.7	1.9
DP4+ (*^{1}H data*)	1.0	0.0	98.9	0.2
DP4+ (*^{13}C data*)	0.0	0.0	97.4	2.5
DP4+ (*all data*)	0.0	0.0	100.0	0.0

Cartesian coordinates (Angstroms) of main conformers of **1**-**4**, optimized at the M06-2X/pecG-2 level in the liquid phase of chloroform, modulated within the IEF-PCM scheme:

Compound: conformer «**1a**»



Imaginary frequencies: none

E^0: -1843.9111954 a.u.

symmetry c1

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C	-4.859806000	1.510625000	0.577402000
N	-4.053683000	1.810429000	1.761917000
C	-4.739742000	1.178960000	2.898332000
C	-5.557130000	0.006132000	2.293821000
C	-5.250688000	0.040461000	0.776157000
C	-6.389158000	-0.494514000	-0.054804000
C	-7.579110000	0.082277000	-0.445158000
C	-8.495127000	-0.675590000	-1.177371000
C	-8.205442000	-1.995610000	-1.494439000
C	-7.009373000	-2.590940000	-1.099689000
C	-6.105996000	-1.825279000	-0.378386000
C	-4.103980000	1.814275000	-0.697705000
C	-2.843545000	0.949599000	-0.720924000
C	-3.295284000	-0.525991000	-0.824131000
C	-2.173605000	-1.523029000	-1.119796000
C	0.224647000	0.924065000	-0.480287000
C	-0.586034000	1.221100000	0.538779000

C	-2.038005000	1.269615000	0.520662000
C	-2.689493000	1.613107000	1.649483000
N	5.957130000	0.405910000	1.283985000
C	4.681319000	0.566408000	0.562376000
C	3.316932000	-1.106582000	-0.871741000
N	1.980147000	-0.680196000	-0.454797000
C	1.841154000	-1.319182000	0.860732000
C	3.259948000	-1.359660000	1.499716000
C	4.212724000	-0.905989000	0.365130000
C	5.530741000	-1.638614000	0.348683000
C	5.846248000	-2.917431000	-0.062858000
C	7.161012000	-3.369045000	0.060555000
C	8.132809000	-2.536137000	0.598702000
C	7.824523000	-1.247088000	1.025762000
C	6.514416000	-0.810916000	0.894538000
C	3.792142000	-0.411052000	-2.121388000
C	3.837879000	1.073864000	-1.832930000
C	4.873403000	1.370865000	-0.739168000
C	4.835875000	2.863486000	-0.434078000
C	1.331690000	3.827328000	-0.719674000
C	2.586951000	3.088289000	-1.131040000
C	2.436503000	1.595825000	-1.476452000
C	1.719123000	0.782534000	-0.377117000
H	-4.378571000	-2.944467000	-0.301657000
H	-3.433989000	-1.103256000	1.245206000
H	-5.767213000	2.117839000	0.636846000
H	-5.404792000	1.899168000	3.371264000
H	-4.011413000	0.853833000	3.635988000
H	-5.297798000	-0.957433000	2.726571000
H	-6.621092000	0.167287000	2.455058000
H	-7.804628000	1.110020000	-0.190303000
H	-9.427752000	-0.235177000	-1.497661000
H	-8.918825000	-2.575830000	-2.062865000
H	-6.791889000	-3.619187000	-1.352459000
H	-3.846049000	2.872401000	-0.726138000
H	-4.741127000	1.596870000	-1.555245000
H	-2.259947000	1.188680000	-1.610801000
H	-3.963714000	-0.571428000	-1.691852000
H	-1.572199000	-1.151091000	-1.954390000
H	-2.607519000	-2.467598000	-1.449435000
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H	-0.129203000	1.450941000	1.499128000
H	-2.137492000	1.791130000	2.565163000
H	6.573052000	1.206011000	1.279959000

H	3.983792000	1.104471000	1.200731000
H	3.249455000	-2.183928000	-1.048787000
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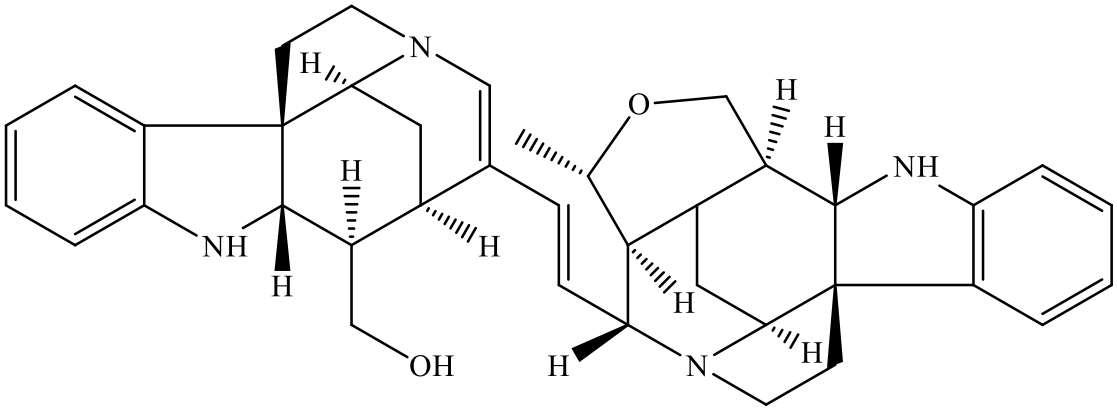
H	1.466877000	-2.332675000	0.719752000
H	3.502888000	-2.371141000	1.818439000
H	3.349313000	-0.712231000	2.369965000
H	5.086014000	-3.566481000	-0.478399000
H	7.423158000	-4.365157000	-0.264263000
H	9.149934000	-2.891239000	0.688185000
H	8.585762000	-0.605043000	1.446312000
H	3.110941000	-0.626430000	-2.945144000
H	4.781049000	-0.783830000	-2.393234000
H	4.157670000	1.614632000	-2.727606000
H	5.857349000	1.116772000	-1.144304000
H	5.476002000	3.121352000	0.409785000
H	5.176765000	3.432783000	-1.306587000
H	1.544261000	4.893070000	-0.663685000
H	0.530602000	3.661269000	-1.437722000
H	0.989259000	3.491069000	0.255535000
H	2.992625000	3.565759000	-2.033464000
H	1.832137000	1.530174000	-2.386257000
H	2.034830000	1.177564000	0.596687000
O	-1.352990000	-1.837422000	-0.012165000
O	3.529228000	3.271728000	-0.080826000
H	-0.728499000	-1.114481000	0.115544000

Compound: conformer «**2b**»



Imaginary frequencies: none

E^0: -1843.9135375 a.u.

symmetry c1

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C	-4.929249000	1.557089000	0.309551000
N	-4.237042000	2.107167000	1.477460000
C	-4.968680000	1.622202000	2.657940000
C	-5.700461000	0.332015000	2.199872000
C	-5.259902000	0.121639000	0.732628000
C	-6.287523000	-0.615979000	-0.085140000
C	-7.465563000	-0.188562000	-0.661991000
C	-8.263753000	-1.110292000	-1.340401000
C	-7.872431000	-2.440068000	-1.420847000
C	-6.689516000	-2.883501000	-0.835222000
C	-5.903541000	-1.955749000	-0.168850000
C	-4.099825000	1.667107000	-0.949162000
C	-2.784820000	0.929179000	-0.722302000
C	-3.083424000	-0.576536000	-0.537152000
C	-1.824187000	-1.418848000	-0.344783000
C	0.194505000	1.223793000	-0.388289000
C	-0.646164000	1.527307000	0.601068000
C	-2.098191000	1.528920000	0.486179000
C	-2.855163000	1.993513000	1.497187000
N	5.773821000	0.055707000	1.476743000
C	4.538411000	0.392203000	0.744414000
C	3.100534000	-1.023542000	-0.892578000
N	1.779876000	-0.539782000	-0.469146000
C	1.557703000	-1.271547000	0.791193000
C	2.950321000	-1.503460000	1.440562000
C	3.965705000	-1.011389000	0.381072000
C	5.225011000	-1.839299000	0.317759000

C	5.456633000	-3.087741000	-0.222652000
C	6.728651000	-3.651512000	-0.117375000
C	7.742491000	-2.958983000	0.531125000
C	7.518628000	-1.702385000	1.087010000
C	6.249826000	-1.153350000	0.972764000
C	3.677617000	-0.245063000	-2.048685000
C	3.836462000	1.198180000	-1.614900000
C	4.836142000	1.311630000	-0.457874000
C	4.875447000	2.767696000	-0.005927000
C	2.923366000	4.238502000	-1.768784000
C	2.621073000	3.201666000	-0.696728000
C	2.465833000	1.780880000	-1.257336000
C	1.657615000	0.932607000	-0.256603000
H	-4.128020000	-2.915326000	0.182512000
H	-3.470268000	-0.813482000	1.572140000
H	-5.869873000	2.103857000	0.198234000
H	-4.273871000	1.446600000	3.474934000
H	-5.689558000	2.371192000	2.981176000
H	-6.778176000	0.478884000	2.236477000
H	-5.461548000	-0.532624000	2.815356000
H	-7.769968000	0.848230000	-0.594894000
H	-9.184228000	-0.789151000	-1.805309000
H	-8.494272000	-3.147306000	-1.951711000
H	-6.390806000	-3.920226000	-0.903678000
H	-3.914832000	2.715512000	-1.180580000
H	-4.654918000	1.229371000	-1.779876000
H	-2.158998000	1.032493000	-1.606002000
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H	-1.281009000	-1.045139000	0.525820000
H	-0.191084000	1.025590000	-1.380989000
H	-0.240258000	1.738992000	1.588269000
H	-2.392526000	2.354227000	2.409237000
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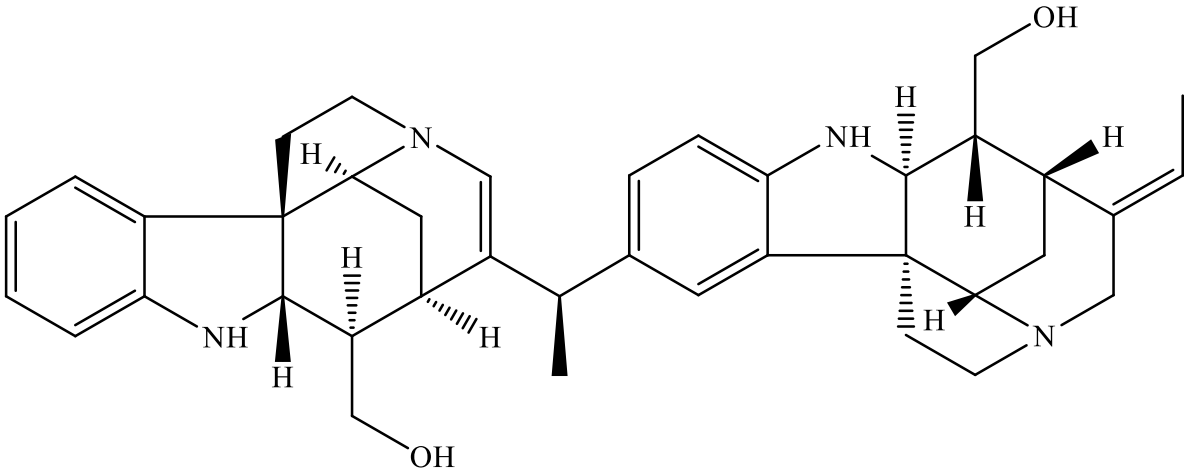
H	1.090046000	-2.230335000	0.562671000
H	3.100564000	-2.561553000	1.644428000
H	3.070419000	-0.968836000	2.380678000
H	4.664570000	-3.626895000	-0.726752000
H	6.924839000	-4.624750000	-0.542734000
H	8.726568000	-3.400231000	0.606859000
H	8.312439000	-1.170161000	1.592417000

H	3.016079000	-0.318404000	-2.912640000
H	4.642126000	-0.674491000	-2.324901000
H	4.241171000	1.781865000	-2.444380000
H	5.820889000	1.036689000	-0.847430000
H	5.493948000	2.895371000	0.883056000
H	5.299162000	3.394514000	-0.796537000
H	3.104990000	5.206603000	-1.305726000
H	3.789088000	3.977846000	-2.374716000
H	2.067088000	4.329411000	-2.434965000
H	1.689543000	3.483344000	-0.204073000
H	1.887186000	1.840574000	-2.183416000
H	1.985290000	1.197897000	0.754423000
O	-1.001375000	-1.412309000	-1.495680000
O	3.585314000	3.225135000	0.357129000
H	-0.102187000	-1.140990000	-1.253149000

Compound: conformer «**3b**»



Imaginary frequencies: none

E^0: -1845.1014972 a.u.

symmetry c1

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N	-4.168371000	-2.622078000	0.007695000
C	-5.337845000	-3.025710000	-0.777385000
C	-6.160535000	-1.734117000	-1.025149000
C	-5.452975000	-0.632265000	-0.188354000
C	-6.458062000	0.325566000	0.402077000
C	-7.294030000	0.195803000	1.494994000
C	-8.214441000	1.207175000	1.766485000
C	-8.296575000	2.321274000	0.941757000
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C	-3.446404000	-0.755493000	1.428818000
C	-2.568797000	-0.219509000	0.301690000
C	-3.322198000	0.883523000	-0.463911000
C	-3.535793000	2.118663000	0.420516000
C	-0.640310000	-2.291433000	-2.419880000
C	-0.871830000	-1.223079000	-1.351060000
C	-2.181094000	-1.360162000	-0.612592000
C	-2.987730000	-2.418016000	-0.726153000
N	3.666486000	-0.937159000	2.062324000
C	4.590662000	-0.127848000	1.246136000
C	4.208113000	1.031135000	-1.067941000
N	4.966737000	2.269197000	-0.878919000
C	4.049109000	3.073610000	-0.066107000
C	3.312906000	2.089734000	0.889273000

C	3.622602000	0.677740000	0.318723000
C	2.423358000	-0.237790000	0.273369000
C	1.326454000	-0.237377000	-0.566028000
C	0.309660000	-1.179627000	-0.393308000
C	0.425264000	-2.102613000	0.642464000
C	1.517826000	-2.109528000	1.504285000
C	2.515859000	-1.165926000	1.308754000
C	5.024814000	-0.064022000	-1.710615000
C	6.189736000	-0.405150000	-0.783888000
C	5.610998000	-1.018408000	0.510168000
C	6.708119000	-1.491477000	1.463860000
C	9.280027000	-0.152496000	-1.199698000
C	8.322886000	0.942570000	-0.840906000
C	7.011156000	0.853810000	-0.614557000
C	6.242384000	2.075737000	-0.169918000
H	-5.930854000	1.391799000	-2.355872000
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H	-1.453403000	-2.309845000	-3.145073000
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H	4.068595000	-1.736608000	2.528686000
H	5.132826000	0.543339000	1.906207000
H	3.364934000	1.286858000	-1.714709000
H	3.329904000	3.552539000	-0.729248000
H	4.591988000	3.856231000	0.459003000
H	3.654954000	2.175582000	1.918863000
H	2.242478000	2.282387000	0.885405000

H	1.242933000	0.492986000	-1.363345000
H	-0.363857000	-2.831088000	0.782530000
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H	9.745515000	0.048826000	-2.164911000
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H	-4.447386000	3.087052000	-0.950516000
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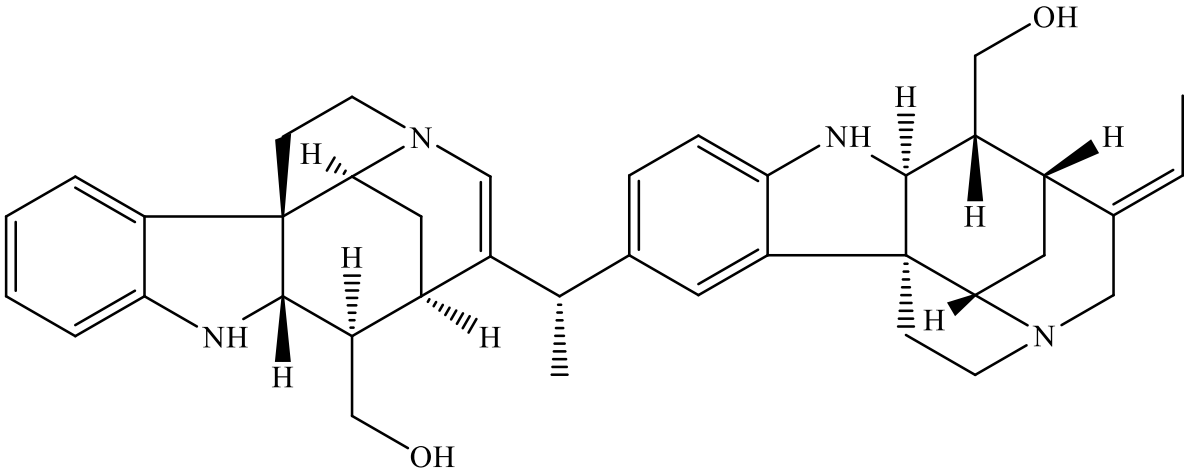
Compound: conformer «**4c**»



Imaginary frequencies: none

E^0: -1845.0991676 a.u.

symmetry c1

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C	-4.382317000	-0.648853000	2.344470000
C	-4.874112000	-0.079749000	0.993808000
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C	1.435856000	0.673744000	-0.551632000
C	0.269921000	0.067974000	-1.023113000
C	0.152309000	-1.317000000	-0.907283000
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C	2.294313000	-1.475070000	0.121576000
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C	6.204629000	-0.143964000	-1.057166000
C	5.423805000	-1.363443000	-0.519805000
C	6.342267000	-2.547991000	-0.219406000
C	9.319601000	-0.235557000	-1.335659000
C	8.526222000	0.459049000	-0.271649000
C	7.202737000	0.476777000	-0.104960000
C	6.608010000	1.166132000	1.100496000
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H	-0.155573000	2.877339000	-1.342837000
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H	5.220064000	2.268382000	2.872481000
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H	2.612072000	1.301295000	2.195758000

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H	9.904595000	0.485628000	-1.906976000
H	9.121075000	1.000598000	0.457542000
H	7.365475000	1.790220000	1.572746000
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O	-6.332356000	0.849485000	-2.171507000
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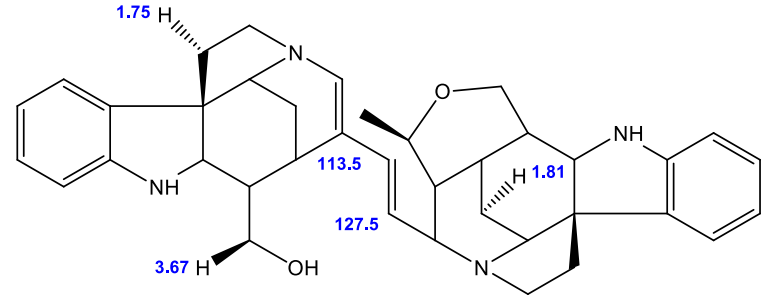
Figure S2. Missing NMR chemical shifts of **1**-**3**. Blue numbers: calculated NMR chemical shifts.



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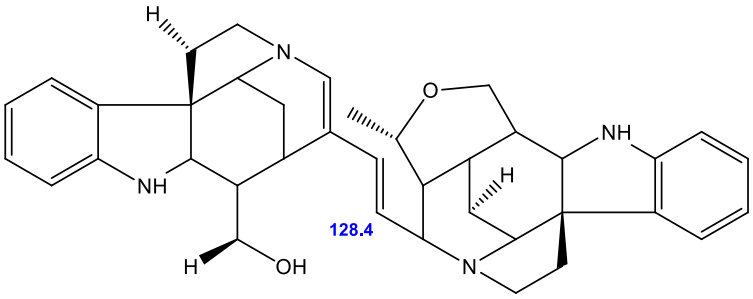

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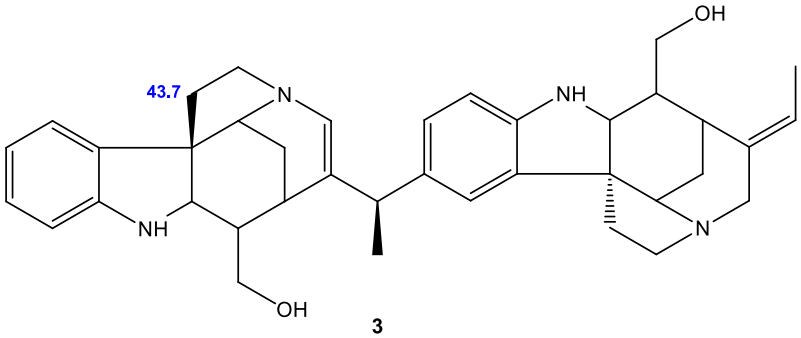

3