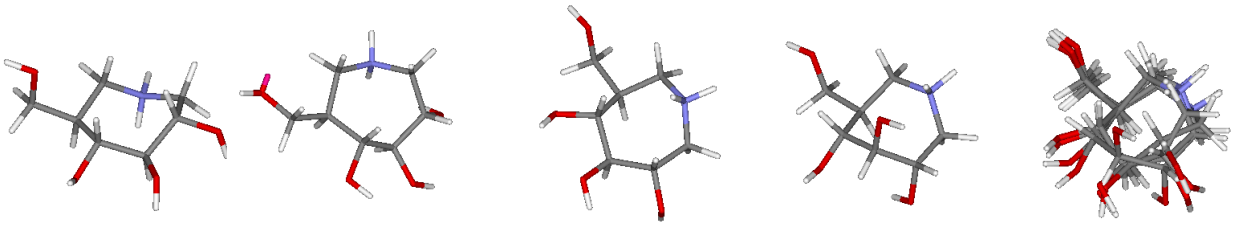
Electronic Supplementary Material (ESI) for New Journal of Chemistry

SUPPLEMENTARY MATERIAL

Compound 1

Conformers **A1**, **B1**, **C1** and **D1** are displayed as well as the superimposition of the four conformers.



D1 **C1** **B1** **A1** **A1/B1/C1/D1**

NMR data:

Chemical shifts for azepane **1** (D_2O, 500 MHz, 300 K):

H	δ (ppm)
H1a	3.28
H1b	3.22
H2	3.97
H3	3.66
H4	3.51
H5	2.11
H6ab	3.74/3.62
H7ab	3.40/3.01

NOE data:

	NOE	distance
H4-H2	w	3.2
H3-H1	w	3.2
H2-H7	mw	3.0
H3-H5	ms	2.7
H1-H7	ms	2.6
H4-H7	m	2.7

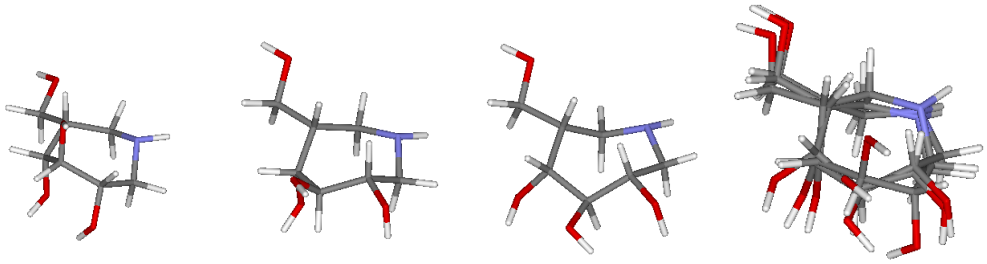
Distances calculated with NOEPROM of MM3 conformers:

	A1	**B1**	**C1**	**D1**	Exp. distance
H4-H2	4.3	2.7	2.8	2.4	3.2
H3-H1	4.2	2.9	3.8	2.9	3.2
H2-H7	4.7	4.3	4.3	2.5	3.0
H3-H5	3.7	2.3	2.3	2.8	2.7
H1-H7	2.8	2.6	2.3	2.7	2.6

H4-H7	2.9	2.8	2.7	2.7	2.7

Compound 2

Conformers **A2**, **B2**, and **C2** are displayed as well as the superimposition of the three conformers.



C2 **B2** **A2** **A2/B2/C2**

NMR data:

Chemical shifts for azepane **2** (D_2O, 500 MHz, 300 K):

H	δ (ppm)
H1ab	3.31/3.29
H2	3.99
H3	3.98
H4	3.90
H5	2.35
H6ab	3.55/3.53
H7ab	3.20/3.18

NOE data:

	NOE	distance
H2-H4	ov	3.0
H3-H1	m	2.8
H2-H5	ov	3.0
H3-H7	vw	3.5
H1-H7	m	2.6

Distances calculated with NOEPROM of MM3 conformers:

	A2	**B2**	**C2**	Exp. distance
H2-H4	2.7	3.8	4.3	3.0
H3-H1	2.3	2.8	3.9	2.8
H2-H5	2.3	2.4	4.1	3.0
H3-H7	2.6	4.2	3.7	3.5

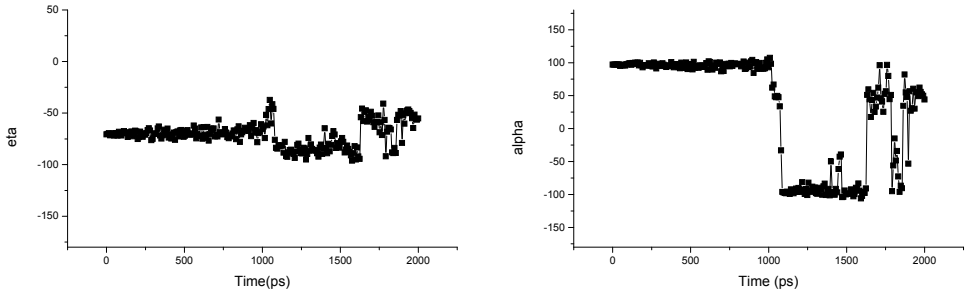
H1-H7	2.5	2.6	2.3	2.6

Compound 3

Conformers **A3** and **B3** are displayed.

A3 **B3**

Trajectory of the MD simulation (MM3*) for azepane **3** starting from conformer **A3**. The oscillation in values of two of the torsion angles of the 7-membered rings are given. In particular, alpha torsion corresponds to C2-N3-C4-C5 dihedral angle and eta torsion to C6-C7-C1-C2 dihedral angle.



NMR data:

Chemical shifts for azepane **3** (D_2O, 500 MHz, 300 K):

H	δ (ppm)
H1a	3.315
H1b	3.306
H2	4.005
H3	3.612
H4	3.346
H5	2.145
Me-6	1.066
H7b	3.263
H7a	2.941

NOE data:

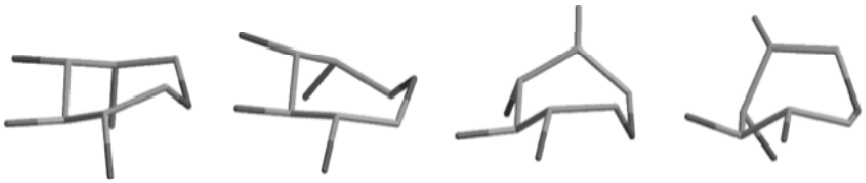
	noe	distance
H2a-H3	vw	3.5
H2b-H3	m	2.9
H3-H4	w	3.3
H3-H5	m	2.9
H3-H6	vvw	4
H4-H2a	ms	2.7
H4-H6	w	3.3
H5-H2a	vvw	4
H5-H6	m	2.9
H6-H2a	vw	3.5
H7a-H2a	m	2.8
H7a-H6	m	2.9
H7b-H2a	m	2.9
H7b-H6	ms	2.8

Distances calculated with NOEPROM of MM3 conformers:

	A3	**B3**	Exp. distance
H2a-H3	3.05	2.32	3.5
H2b-H3	2.37	2.61	2.9
H3-H4	3.07	3.07	3.3
H3-H5	2.29	2.74	2.9
H3-H6	4.57	4.61	4
H4-H2a	2.79	3.73	2.7
H4-H6	2.75	2.35	3.3
H5-H2a	4.03	2.50	4
H5-H6	3.03	3.12	2.9
H6-H2a	4.22	4.10	3.5
H7a-H2a	2.19	3.54	2.8
H7a-H6	2.35	2.44	2.9
H7b-H2a	3.36	2.26	2.9
H7b-H6	2.55	3.09	2.8

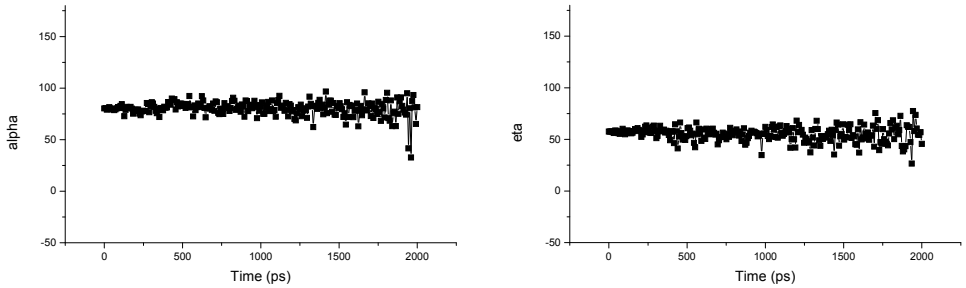
Compound 4

Conformers **A4**, **B4**, **C4** and **D4** are displayed.



A4 **B4** **C4** **D4**

Trajectory of the MD simulation (MM3*) for compound **4** starting from conformer **C4**. The oscillation in values of two of the torsion angles of the seven-membered rings are given. In particular, alpha torsion corresponds to C2-N3-C4-C5 dihedral angle and eta to C6-C7-C1-C2 dihedral angle.



NMR data:
Chemical shifts for azepane **4** (D_2O, 500 MHz, 300 K):

H	δ (ppm)
H1a	3.392
H1b	3.323
H2	4.028
H3	3.901
H4	3.859
H5	2.399
Me-6	1.067
H7a	3.199
H7b	3.114

NOE data:

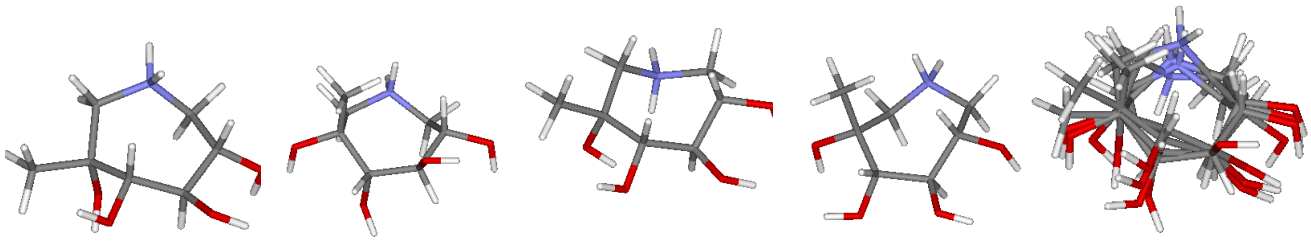
	NOE	distance
H2a-H3	ms	2.8
H2b-H3	mw	3.1
H3-H4	ms	2.8
H3-H5	w	3.3
H3-H6	m	2.9
H4-H2a	vw	3.5
H4-H6	w	3.3
H5-H2a	vw	3.5
H5-H2b	vw	3.5
H5-H6	m	2.9
H6-H2a	vvw	4
H7a-H5	vw	3.5
H7a-H6	w	3.3
H7b-H2a	m	3.5
H7b-H6	m	2.9

Distances calculated with NOEPROM of MM3 conformers:

	A4	**B4**	**C4**	**D4**	Exp. distance
H2a-H3	2.40	3.05	2.45	2.96	2.8
H2b-H3	2.49	2.33	3.08	2.31	3.1
H3-H4	2.50	2.35	2.38	2.59	2.8
H3-H5	3.74	3.78	3.61	3.78	3.3
H3-H6	4.87	4.38	2.63	2.21	2.9
H4-H2a	2.66	3.67	4.30	4.06	3.5
H4-H6	2.70	2.36	2.87	3.67	3.3
H5-H2a	4.12	2.56	4.09	4.83	3.5
H5-H2b	4.07	3.98	3.15	4.61	3.5
H5-H6	3.08	3.11	3.11	3.10	2.9
H6-H2a	4.09	4.11	4.39	3.93	4
H7a-H5	3.81	2.79	3.45	2.83	3.5
H7a-H6	2.64	3.09	2.82	3.08	3.3
H7b-H2a	2.18	3.50	2.66	3.68	3.5
H7b-H6	2.33	2.41	2.34	2.42	2.9

Compound 5

Conformers **A5**, **B5**, **C5** and **D5** are displayed as well as the superimposition of the four conformers.



D5 **C5** **B5** **A5** **A5/B5/C5/D5**

NMR data:

Chemical shifts for azepane **5** (D_2O, 500 MHz, 300 K):

H	δ (ppm)
H1a	3.27
H1b	3.16
H2	4.14
H3	3.63
H4	3.67
H7ab	3.27/2.97

NOE data:

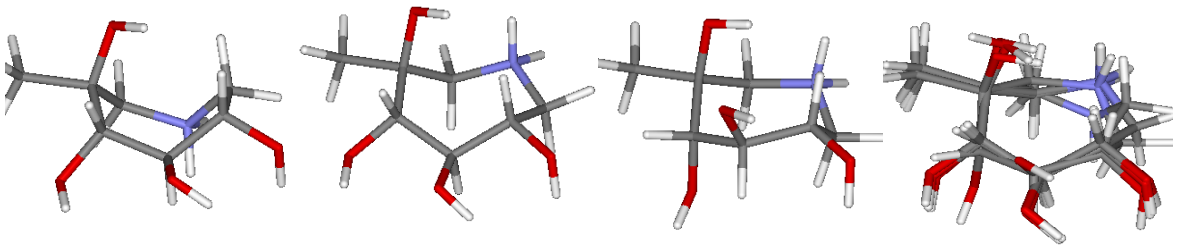
	NOE	distance
Me-H7	s	2.5
H4-H2	mw	3.0
H3-H1	ms	2.8
H4-H7	mw	3.0

Distances calculated with NOEPROM of MM3 conformers:

	A5	**B5**	**C5**	**D5**	Exp. distance
Me-H7	2.5	2.5	2.5	2.6	2.5
H4-H2	2.8	2.4	3.9	2.8	3.0
H3-H1	2.4	2.8	2.9	2.9	2.8
H4 H7	3.9	2.8	3.1	2.8	3.0

Compound 6

Conformers **A6**, **B6** and **C6** are displayed as well as the superimposition of the three conformers.



C6 **B6** **A6** **A6/B6/D6**

NMR data:

Chemical shifts for azepane **6** (D_2O, 500 MHz, 300 K):

H	d (ppm)
H1a	3.31
H1b	3.251
H2	3.900
H3	3.647
H4	3.33
H7ab	3.166
Me	1.067

NOE data:

	NOE	distance
Me-H4	m	2.9
Me-H7	s	2.5
H3-H2	w	3.1
H4-H2	ms	2.7
H3-H4	mw	3.0
H3-H1	ms	2.8
H4 H7	vw	3.7

Distances calculated with NOEPROM of MM3 conformers:

	A6	**B6**	**C6**	Exp. distance
Me-H4	2.9	3.2	2.9	2.9
Me-H7	2.5	2.5	2.5	2.5
H3-H2	3.0	3.1	3.1	3.1
H4-H2	3.9	2.7	2.9	2.7
H3-H4	2.6	3.1	3.1	3.0
H3-H1	3.0	2.4	3.5	2.8
H4 H7	3.7	3.9	4.1	3.7

Figure 6H

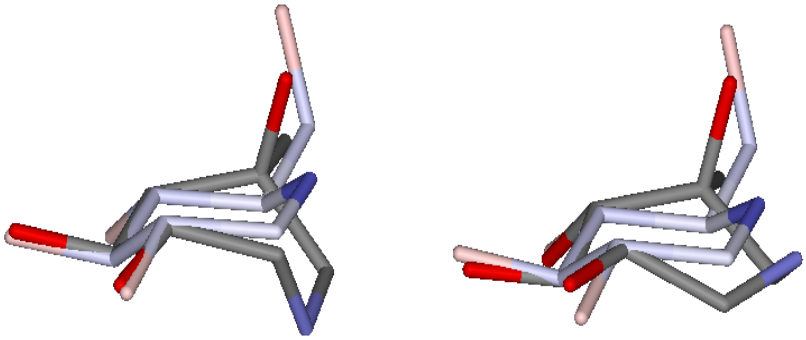


Figure 6I

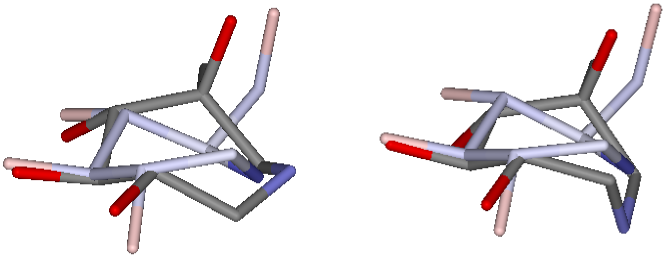


Figure 6J