Electronic Supplementary Information (ESI)

Equilibrium structures of the tetramezine diastereomers and their ratio: joint analysis of gas phase electron diffraction, quantum chemistry, and spectroscopic data

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Contents

1. Synthesis of 1,2-*bis*-(3,3-dimethyldiaziridin-1-yl)ethane (tetramezine).

Commercially available chemicals were purchased from the ACROS catalog and were used as received.

1,2-*bis*-(3,3-dimethyldiaziridin-1-yl)ethane (tetramezine), $\boldsymbol{S_N S_N}$–$\boldsymbol{R_{N'} R_{N'}}$ was for the first time synthesized at the N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciencies (RAS).

22.7 g (0.10 mol) acetone oxime *p*-toluenesulfonate (prepared according to the synthesis of acetone oxime benzenesulfonate by Oxley and Short) were dissolved in 20 ml dichloromethane. At a temperature of 10–15^{o}C, 3.0 g ethylenediamine and 15 g triethylamine were added. The reaction mixture was stirred for 24 h at room temperature and for 4 days at 25–30^{o}C. Then, 40 ml dichloromethane and 15 g finely ground potassium carbonate were added. After stirring the mixture for 5 h, the precipitate was filtered off and washed with 25 ml dichloromethane. After solvent evaporation by arotary evaporator at a bath temperature of 40^{o}C and crystallization from acetone with fast cooling and stirring, 6.2 g of the diastereomeric mixture of tetramezine was collected by filtration. The *meso* form was isolated in high purity by recrystallizing the diastereomeric mixture from acetone under slow cooling and fully characterized by IR, NMR, HR-MS, and X-ray diffraction analysis.

Experimental

The IR spectrum of the *meso*-tetramezine was recorded on a “Nicolet Magna 750” (USA) spectrometer in the range 400-4000 cm^{-1} (resolution 2 cm^{-1}) as pellets with KBr.
IR-spectrum (ν/cm^{-1}, Figure S1): 428, 507, 542, 656, 758, 807, 826, 977, 1004, 1073, 1103, 1127, 1208, 1274, 1301, 1320, 1351, 1383, 1448, 1464, 2863, 2934, 2964, 3006, 3213.

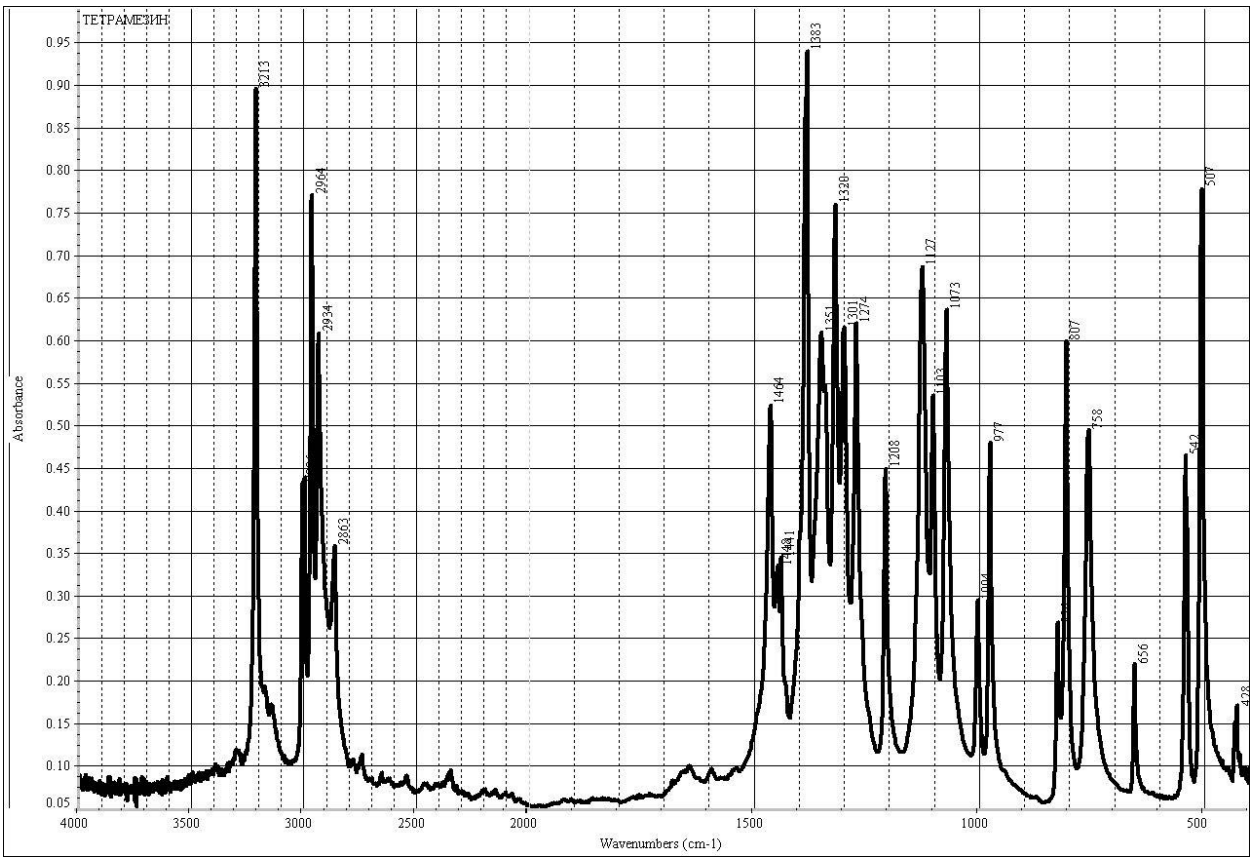

Fig. S1. IR spectrum of crystalline *meso*-form of tetramezine

Mass spectra were measured using a Finnigan MAT INCOS-50 instrument. High resolution mass spectra were recorded on a Bruker microTOF spectrometer with electrospray ionization (ESI). All measurements were performed in a positive (+MS) ion mode (interface capillary voltage: 4500 V) with scan range *m/z*: 50-3000.

HRMS (ESI): m/z for $C_8H_{18}N_4$ $(M+H)^+$: calcd 171.1604, found 171.1608; m/z for $C_8H_{18}N_4$ $[M+Na]^+$: calcd 193.1424, found 193.1427.; Mass-spectra (EI, 70 eV), *m/z*: 170 $[M]^+$, 155 $[M - Me]^+$, 139 $[M - 2Me - H]^+$, 125 $[M - 3Me]^+$, 111 $[M - 4Me + H]^+$, 85 $[M - \text{-}CH_2\text{-N-}C_{ring}(Me_2)\text{-NH}]^+$, 70 $[M - \text{-}CH_2\text{-N-}C_{ring}(Me_2)\text{-NH} - Me]^+$, 56 $[M - \text{-}CH_2\text{-N-}C_{ring}(Me_2)\text{-NH} - 2Me + H]^+$.

2. NMR spectra

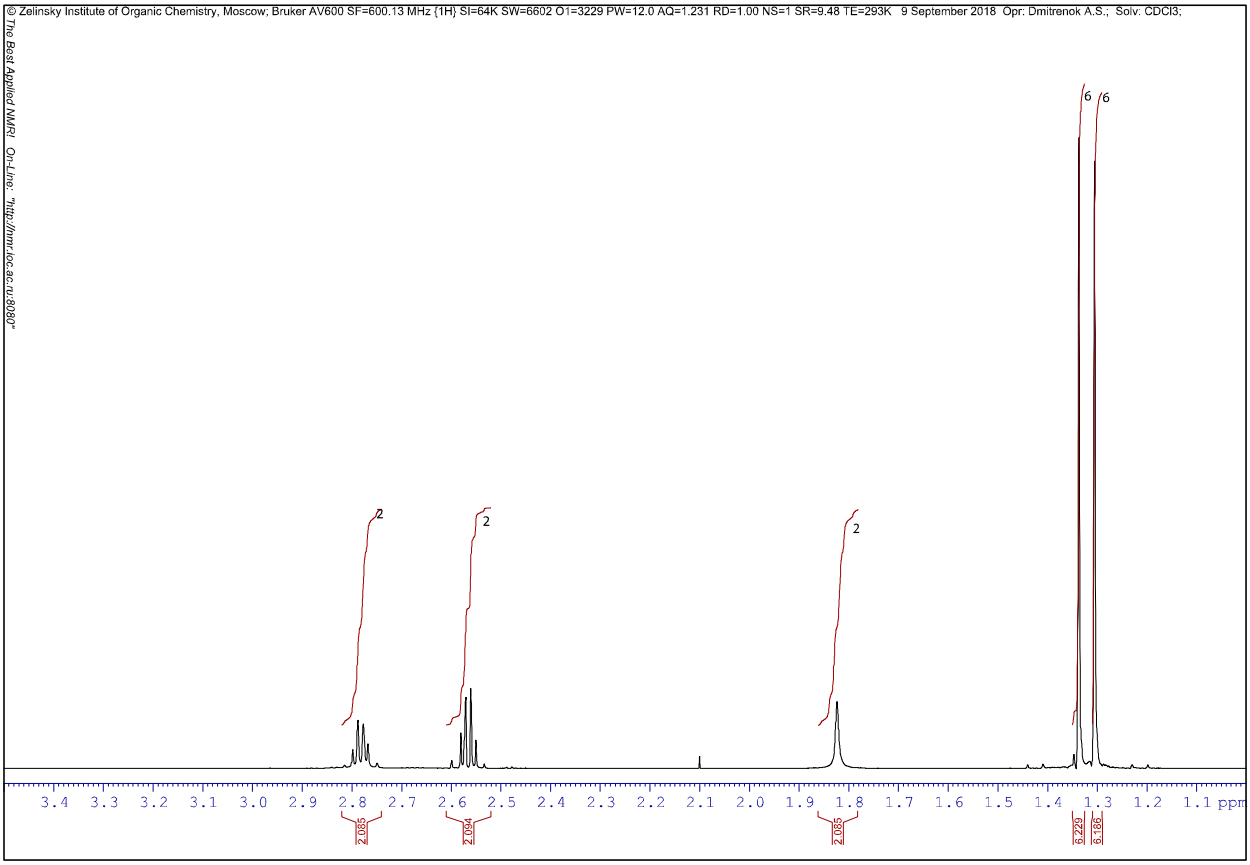

Fig. S2. ^{1}H NMR spectrum of 1,2-*bis*-(3,3-dimethyldiaziridin-1-yl)ethane, S_NS_N–R_NR_N (solution in $CDCl_3$).

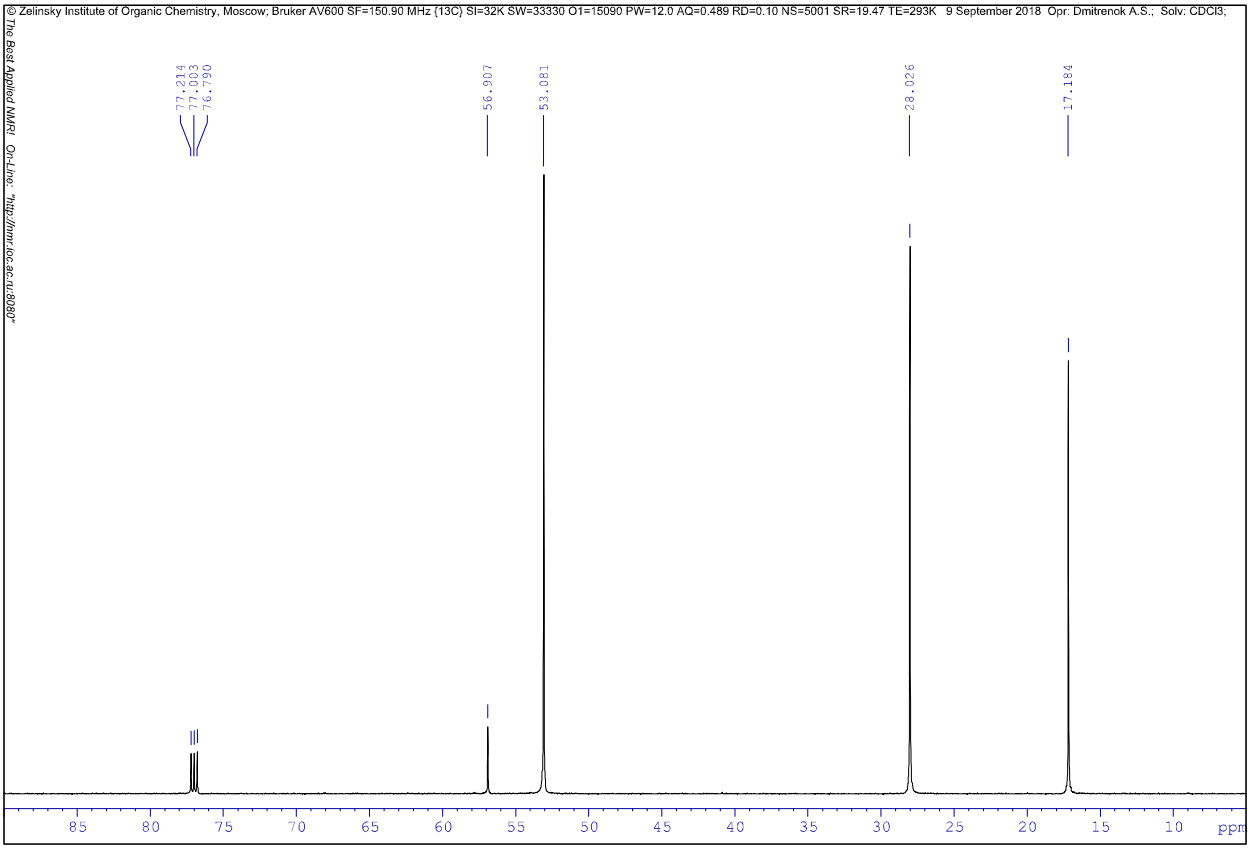

Fig.S3. ^{13}C NMR spectrum of 1,2-*bis*-(3,3-dimethyldiaziridin-1-yl)ethane, S_NS_N–$R_{N'}R_{N'}$ (solution in $CDCl_3$).

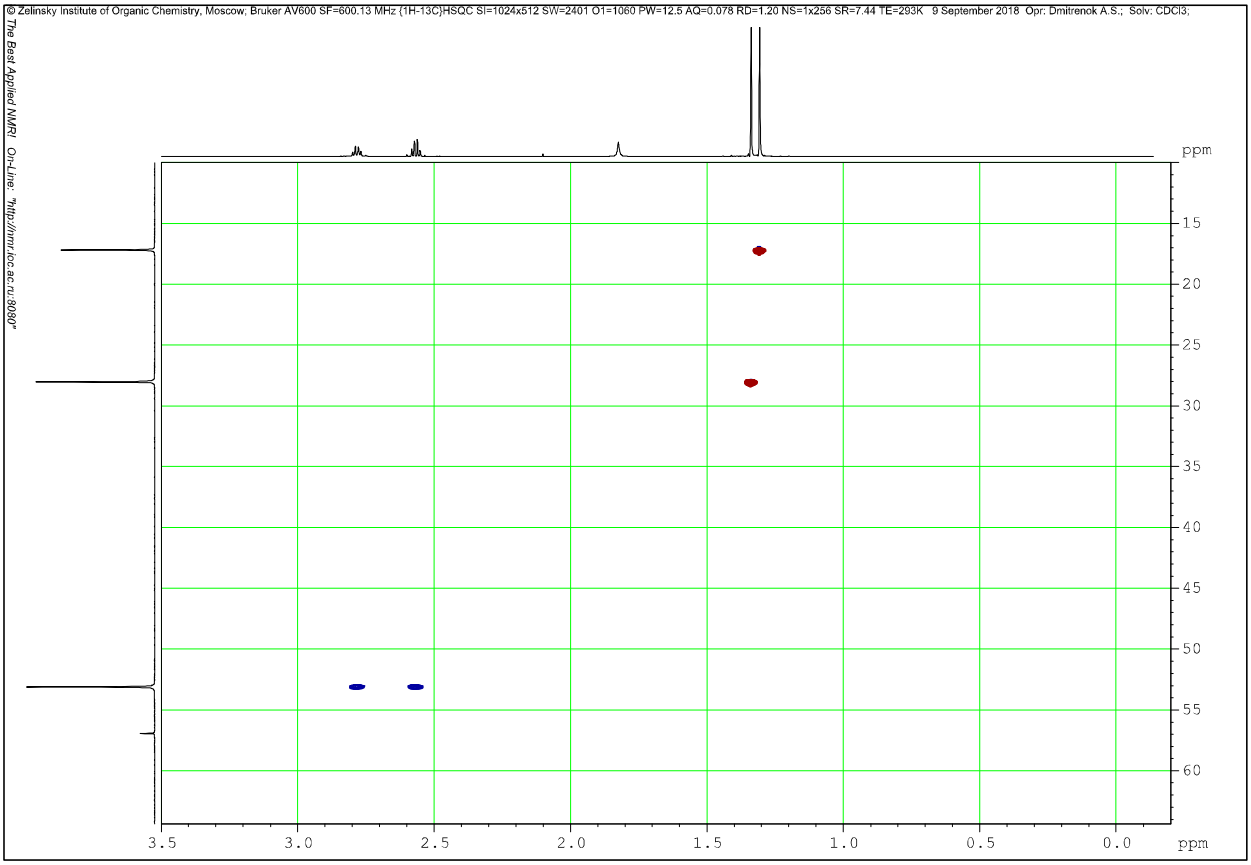

Fig.S4. 2D NMR spectrum {^{1}H-^{13}C} HMBC of 1,2-*bis*-(3,3-dimethyldiaziridin-1-yl)ethane, S_NS_N–$R_N{}'R_N{}'$ (solution in $CDCl_3$).

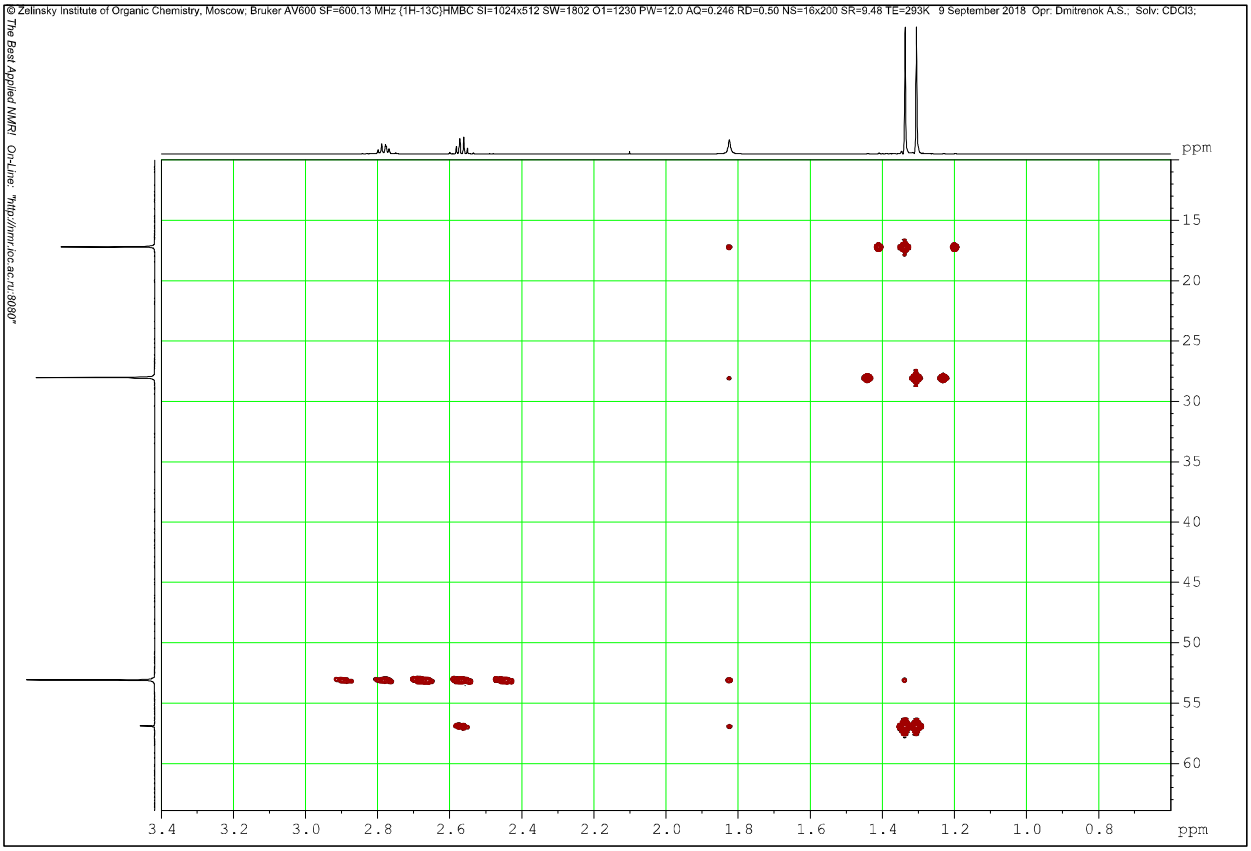

Fig.S5. 2D NMR spectrum {^{1}H-^{13}C} HMBC of 1,2-*bis*-(3,3-dimethyldiaziridin-1-yl)ethane, S_NS_N–$R_{N'}R_{N'}$ (solution in $CDCl_3$).

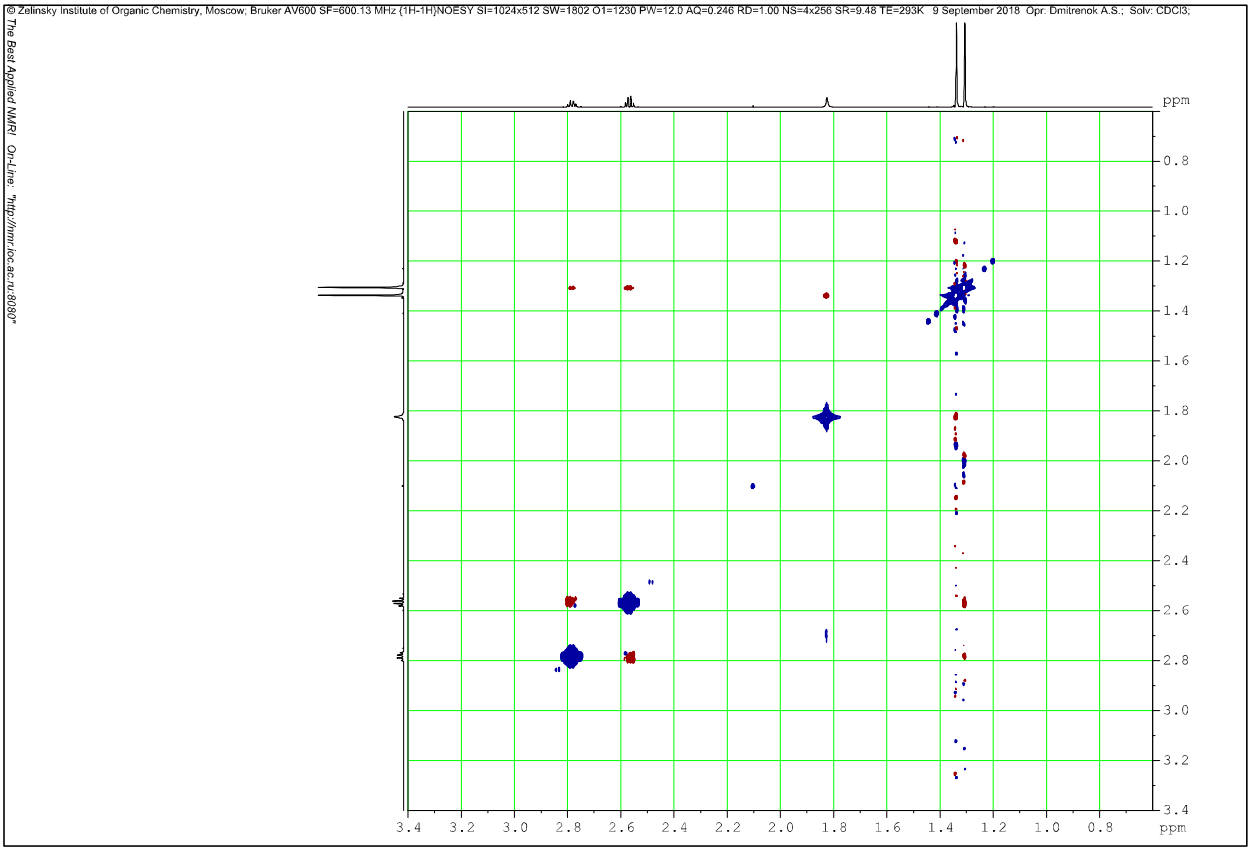

Fig.S6. 2D NMR spectrum {^{1}H-^{1}H}gNOESY of 1,2-*bis*-(3,3-dimethyldiaziridin-1-yl)ethane, S_NS_N–$R_{N'}R_{N'}$ (solution in $CDCl_3$).

3. Interpretation of the experimental IR spectrum

Table S1. Redundant set of internal vibrational coordinates for tetramezine.

№	Notation	Atom group	№	Notation	Atom group
Stretching coordinates			***Bending coordinates***		
1	C1C2	C1–C2	50	H22N20N19	H22–N20–N19
2	C1H3	C1–H3	51	H22N20C21	H22–N20–C21
3	C1H4	C1–H4	52	C9C7C10	C9–C7–C10
4	C1N5	C1–N5	53	N5C7C9	N5–C7–C9
5	N5N6	N5–N6	54	N5C7C10	N5–C7–C10
6	N5C7	N5–C7	55	N6C7C9	N6–C7–C9
7	N6C7	N6–C7	56	N6C7C10	N6–C7–C10
8	N6H8	N6–H8	57	C23C21C24	C23–C21–C24
9	C7C9	C7–C9	58	N19C21C23	N19–C21–C23
10	C7C10	C7–C10	59	N19C21C24	N19–C21–C24
11	C9H11	C9–H11	60	N20C21C23	N20–C21–C23
12	C9H12	C9–H12	61	N20C21C24	N20–C21–C24
13	C9H13	C9–H13	62	C7C9H11	C7–C9–H11
14	C10H14	C10–H14	63	C7C9H12	C7–C9–H12
15	C10H15	C10–H15	64	C7C9H13	C7–C9–H13
16	C10H16	C10–H16	65	C7C10H14	C7–C10–H14
17	C2H17	C2–H17	66	C7C10H15	C7–C10–H15
18	C2H18	C2–H18	67	C7C10H16	C7–C10–H16
19	C2N19	C2–N19	68	H12C9H13	H12–C9–H13
20	N19N20	N19–N20	69	H11C9H13	H11–C9–H13
21	N19C21	N19–C21	70	H11C9H12	H11–C9–H12
22	N20C21	N20–C21	71	H15C10H16	H15–C10–H16
23	N20H22	N20–H22	72	H14C10H16	H14–C10–H16
24	C21C23	C21–C23	73	H14C10H15	H14–C10–H15
25	C21C24	C21–C24	74	C21C23H25	C21–C23–H25
26	C23H25	C23–H25	75	C21C23H26	C21–C23–H26
27	C23H26	C23–H26	76	C21C23H27	C21–C23–H27
28	C23H27	C23–H27	77	C21C24H28	C21–C24–H28
29	C24H28	C24–H28	78	C21C24H29	C21–C24–H29
30	C24H29	C24–H29	79	C21C24H30	C21–C24–H30
31	C24H30	C24–H30	80	H26C23H27	H26–C23–H27
Bending coordinates			81	H25C23H27	H25–C23–H27
32	C2C1H3	C2–C1–H3	82	H25C23H26	H25–C23–H26
33	C2C1H4	C2–C1–H4	83	H29C24H30	H29–C24–H30
34	C2C1N5	C2–C1–N5	84	H28C24H30	H28–C24–H30
35	H3C1H4	H3–C1–H4	85	H28C24H29	H28–C24–H29
36	H3C1N5	H3–C1–N5	***Wagging vibrations (out of plane)***		
37	H4C1N5	H4–C1–N5	86	C1wag	C1–N5 / N5N6C7
38	C1C2H17	C1–C2–H17	87	C2wag	C2–N19 / N19N20C21
39	C1C2H18	C1–C2–H18	88	H8wag	H8–N6 / N6N5C7
40	C1C2N19	C1–C2–N19	89	H22wag	H22–N20 / N20N19C21
41	H17C2H18	H17–C2–H18	***Torsional vibrations***		
42	H17C2N19	H17–C2–N19	90	TC1C2	(H3,H4,N5)C1–C2(N19,H18,H17)
43	H18C2N19	H18–C2–N19	91	TC1N5	(C2,H3,H4)C1–N5(N6,C7)
44	C1N5N6	C1–N5–N6	92	TC2N19	(C1,H17,H18)C2–N19(N20,C21)
45	C1N5C7	C1–N5–C7	93	TC7C9	(N5,N6,C10)C7–C9(H11,H12,H13)
46	C2N19N20	C2–N19–N20	94	TC7C10	(N5,N6,C9)C7–C10(H14,H15,H16)
47	C2N19C21	C2–N19–C21	95	TC21C23	(N19,N20,C24)C21–C23(H25,H26,H27)
48	H8N6N5	H8–N6–N5	96	TC21C24	(N19,N20,C23)C21–C24(H28,H29,H30)
49	H8N6C7	H8–N6–C7			

4. Experimental GED data for structural analysis and the refinement results

Table S2. The total scattering intensity functions $I^{tot}(s)$ and the background lines $I^{b}(s)$ for tetramezine. Long camera distance (LD=362.3 mm).

The used diffraction pattern no.1

S	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$
3.125	0.38574	0.41703	8.500	0.41020	0.39940	13.875	0.33616	0.32526
3.250	0.39919	0.42974	8.625	0.40766	0.39640	14.000	0.33276	0.32474
3.375	0.39972	0.44143	8.750	0.40470	0.39353	14.125	0.32946	0.32428
3.500	0.40285	0.45207	8.875	0.40105	0.39077	14.250	0.32656	0.32390
3.625	0.40119	0.46167	9.000	0.39718	0.38812	14.375	0.32405	0.32358
3.750	0.39969	0.47023	9.125	0.39376	0.38557	14.500	0.32192	0.32332
3.875	0.40125	0.47777	9.250	0.39032	0.38312	14.625	0.32043	0.32312
4.000	0.40353	0.48431	9.375	0.38756	0.38076	14.750	0.31933	0.32296
4.125	0.41363	0.48986	9.500	0.38508	0.37847	14.875	0.31846	0.32286
4.250	0.42264	0.49446	9.625	0.38326	0.37626	15.000	0.31780	0.32279
4.375	0.43881	0.49813	9.750	0.38125	0.37411	15.125	0.31761	0.32275
4.500	0.45617	0.50092	9.875	0.38005	0.37202	15.250	0.31749	0.32273
4.625	0.47417	0.50285	10.000	0.37870	0.36998	15.375	0.31722	0.32273
4.750	0.49240	0.50398	10.125	0.37737	0.36799	15.500	0.31715	0.32275
4.875	0.51246	0.50435	10.250	0.37540	0.36603	15.625	0.31642	0.32276
5.000	0.53625	0.50400	10.375	0.37262	0.36412	15.750	0.31553	0.32277
5.125	0.55825	0.50300	10.500	0.36860	0.36223	15.875	0.31465	0.32276
5.250	0.57478	0.50139	10.625	0.36303	0.36038	16.000	0.31370	0.32275
5.375	0.58443	0.49923	10.750	0.35683	0.35855	16.125	0.31334	0.32271
5.500	0.58783	0.49659	10.875	0.35006	0.35674	16.250	0.31282	0.32264
5.625	0.58277	0.49351	11.000	0.34373	0.35496	16.375	0.31273	0.32255
5.750	0.57088	0.49005	11.125	0.33776	0.35320	16.500	0.31360	0.32244
5.875	0.55410	0.48628	11.250	0.33288	0.35146	16.625	0.31468	0.32230
6.000	0.53354	0.48224	11.375	0.32917	0.34975	16.750	0.31601	0.32214
6.125	0.51120	0.47798	11.500	0.32624	0.34807	16.875	0.31784	0.32196
6.250	0.48846	0.47356	11.625	0.32484	0.34641	17.000	0.31967	0.32178
6.375	0.46729	0.46902	11.750	0.32441	0.34479	17.125	0.32154	0.32160
6.500	0.44795	0.46440	11.875	0.32493	0.34320	17.250	0.32346	0.32144
6.625	0.43295	0.45973	12.000	0.32629	0.34164	17.375	0.32526	0.32131
6.750	0.42174	0.45506	12.125	0.32827	0.34013	17.500	0.32708	0.32123
6.875	0.41343	0.45041	12.250	0.33088	0.33867	17.625	0.32832	0.32122
7.000	0.40772	0.44581	12.375	0.33372	0.33725	17.750	0.32960	0.32129
7.125	0.40444	0.44128	12.500	0.33702	0.33589	17.875	0.33076	0.32148
7.250	0.40289	0.43684	12.625	0.33998	0.33458	18.000	0.33135	0.32180
7.375	0.40354	0.43250	12.750	0.34296	0.33333	18.125	0.33224	0.32228
7.500	0.40494	0.42828	12.875	0.34521	0.33215	18.250	0.33294	0.32294
7.625	0.40668	0.42419	13.000	0.34685	0.33103	18.375	0.33307	0.32381
7.750	0.40885	0.42023	13.125	0.34775	0.32999	18.500	0.33308	0.32491
7.875	0.41091	0.41641	13.250	0.34772	0.32901	18.625	0.33299	0.32626
8.000	0.41230	0.41273	13.375	0.34702	0.32811	18.750	0.33268	0.32787
8.125	0.41301	0.40919	13.500	0.34524	0.32729	18.875	0.33298	0.32975
8.250	0.41289	0.40579	13.625	0.34262	0.32654	19.000	0.33323	0.33191
8.375	0.41194	0.40253	13.750	0.33960	0.32586			

The used diffraction pattern no.2

s	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$
3.125	0.38605	0.41842	8.500	0.40685	0.39593	13.875	0.32951	0.31883
3.250	0.39892	0.43014	8.625	0.40399	0.39290	14.000	0.32597	0.31818
3.375	0.39949	0.44102	8.750	0.40115	0.38998	14.125	0.32252	0.31759
3.500	0.40151	0.45103	8.875	0.39763	0.38717	14.250	0.31961	0.31706
3.625	0.39942	0.46015	9.000	0.39331	0.38447	14.375	0.31714	0.31658
3.750	0.39827	0.46837	9.125	0.39000	0.38186	14.500	0.31513	0.31616
3.875	0.39909	0.47567	9.250	0.38669	0.37934	14.625	0.31344	0.31579
4.000	0.40169	0.48205	9.375	0.38364	0.37691	14.750	0.31234	0.31545
4.125	0.41091	0.48751	9.500	0.38123	0.37455	14.875	0.31127	0.31516
4.250	0.42030	0.49205	9.625	0.37929	0.37226	15.000	0.31070	0.31490
4.375	0.43606	0.49571	9.750	0.37723	0.37003	15.125	0.31002	0.31467
4.500	0.45306	0.49848	9.875	0.37580	0.36786	15.250	0.30957	0.31446
4.625	0.47144	0.50041	10.000	0.37443	0.36573	15.375	0.30883	0.31427
4.750	0.48966	0.50153	10.125	0.37313	0.36366	15.500	0.30844	0.31409
4.875	0.51022	0.50188	10.250	0.37090	0.36162	15.625	0.30775	0.31392
5.000	0.53388	0.50151	10.375	0.36807	0.35962	15.750	0.30645	0.31375
5.125	0.55551	0.50046	10.500	0.36386	0.35765	15.875	0.30527	0.31358
5.250	0.57229	0.49880	10.625	0.35864	0.35571	16.000	0.30411	0.31341
5.375	0.58210	0.49659	10.750	0.35238	0.35380	16.125	0.30338	0.31324
5.500	0.58534	0.49388	10.875	0.34527	0.35192	16.250	0.30292	0.31306
5.625	0.57981	0.49073	11.000	0.33874	0.35006	16.375	0.30317	0.31288
5.750	0.56844	0.48720	11.125	0.33268	0.34823	16.500	0.30384	0.31270
5.875	0.55134	0.48336	11.250	0.32771	0.34643	16.625	0.30499	0.31252
6.000	0.53069	0.47925	11.375	0.32396	0.34466	16.750	0.30654	0.31235
6.125	0.50844	0.47493	11.500	0.32124	0.34291	16.875	0.30811	0.31219
6.250	0.48523	0.47046	11.625	0.31962	0.34120	17.000	0.31010	0.31205
6.375	0.46410	0.46586	11.750	0.31931	0.33952	17.125	0.31220	0.31195
6.500	0.44442	0.46120	11.875	0.31980	0.33788	17.250	0.31397	0.31189
6.625	0.43003	0.45650	12.000	0.32134	0.33628	17.375	0.31595	0.31188
6.750	0.41869	0.45180	12.125	0.32322	0.33472	17.500	0.31793	0.31195
6.875	0.41045	0.44713	12.250	0.32582	0.33320	17.625	0.31963	0.31210
7.000	0.40445	0.44251	12.375	0.32846	0.33174	17.750	0.32061	0.31235
7.125	0.40117	0.43797	12.500	0.33154	0.33032	17.875	0.32197	0.31271
7.250	0.39943	0.43352	12.625	0.33435	0.32896	18.000	0.32272	0.31320
7.375	0.40001	0.42917	12.750	0.33708	0.32766	18.125	0.32341	0.31383
7.500	0.40137	0.42495	12.875	0.33905	0.32642	18.250	0.32408	0.31461
7.625	0.40332	0.42085	13.000	0.34065	0.32524	18.375	0.32387	0.31555
7.750	0.40545	0.41688	13.125	0.34158	0.32413	18.500	0.32403	0.31665
7.875	0.40743	0.41305	13.250	0.34149	0.32308	18.625	0.32416	0.31790
8.000	0.40892	0.40936	13.375	0.34051	0.32209	18.750	0.32398	0.31930
8.125	0.40967	0.40580	13.500	0.33876	0.32118	18.875	0.32423	0.32081
8.250	0.40931	0.40238	13.625	0.33614	0.32033	19.000	0.32466	0.32239
8.375	0.40865	0.39909	13.750	0.33308	0.31955			

Table S3. The total scattering intensity functions $I^{tot}(s)$ and the background lines $I^{b}(s)$ for tetramezine. Short camera distance (SD=193.3 mm).

The used diffraction pattern no.1

s	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$
7.00	0.23992	0.25646	15.25	0.19391	0.19624	23.50	0.18805	0.18812
7.25	0.23919	0.25374	15.50	0.19287	0.19539	23.75	0.18801	0.18834
7.50	0.24013	0.25156	15.75	0.19143	0.19457	24.00	0.18796	0.18858
7.75	0.24509	0.24959	16.00	0.18984	0.19378	24.25	0.18797	0.18886
8.00	0.24753	0.24762	16.25	0.18880	0.19302	24.50	0.18831	0.18917
8.25	0.24907	0.24555	16.50	0.18847	0.19230	24.75	0.18884	0.18952
8.50	0.24904	0.24331	16.75	0.18904	0.19162	25.00	0.18976	0.18991
8.75	0.24595	0.24092	17.00	0.19034	0.19099	25.25	0.19040	0.19034
9.00	0.24149	0.23839	17.25	0.19154	0.19040	25.50	0.19134	0.19082
9.25	0.23805	0.23577	17.50	0.19240	0.18986	25.75	0.19196	0.19134
9.50	0.23562	0.23311	17.75	0.19311	0.18936	26.00	0.19247	0.19191
9.75	0.23362	0.23044	18.00	0.19308	0.18892	26.25	0.19312	0.19252
10.00	0.23159	0.22782	18.25	0.19245	0.18853	26.50	0.19364	0.19318
10.25	0.23027	0.22527	18.50	0.19131	0.18818	26.75	0.19421	0.19388
10.50	0.22670	0.22282	18.75	0.18979	0.18789	27.00	0.19471	0.19461
10.75	0.22036	0.22050	19.00	0.18808	0.18764	27.25	0.19536	0.19539
11.00	0.21357	0.21831	19.25	0.18647	0.18743	27.50	0.19595	0.19620
11.25	0.20765	0.21626	19.50	0.18554	0.18727	27.75	0.19655	0.19704
11.50	0.20423	0.21435	19.75	0.18500	0.18714	28.00	0.19750	0.19790
11.75	0.20300	0.21257	20.00	0.18496	0.18705	28.25	0.19823	0.19880
12.00	0.20360	0.21092	20.25	0.18528	0.18700	28.50	0.19923	0.19972
12.25	0.20526	0.20938	20.50	0.18566	0.18697	28.75	0.20035	0.20067
12.50	0.20827	0.20795	20.75	0.18603	0.18697	29.00	0.20119	0.20166
12.75	0.21107	0.20661	21.00	0.18643	0.18699	29.25	0.20256	0.20268
13.00	0.21280	0.20536	21.25	0.18695	0.18703	29.50	0.20389	0.20375
13.25	0.21298	0.20417	21.50	0.18715	0.18708	29.75	0.20498	0.20487
13.50	0.21142	0.20304	21.75	0.18768	0.18716	30.00	0.20650	0.20605
13.75	0.20850	0.20196	22.00	0.18800	0.18725	30.25	0.20780	0.20730
14.00	0.20452	0.20093	22.25	0.18844	0.18735	30.50	0.20907	0.20862
14.25	0.20094	0.19993	22.50	0.18845	0.18747	30.75	0.21048	0.21001
14.50	0.19806	0.19897	22.75	0.18847	0.18760	31.00	0.21181	0.21145
14.75	0.19624	0.19803	23.00	0.18826	0.18776	31.25	0.21302	0.21291
15.00	0.19484	0.19712	23.25	0.18821	0.18793	31.50	0.21426	0.21432
						31.75	0.21568	0.21558

The used diffraction pattern no.2

s	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$	s	$I^{tot}(s)$	$I^{b}(s)$
7.00	0.27464	0.29532	15.25	0.21629	0.21913	23.50	0.20962	0.20985
7.25	0.27191	0.29067	15.50	0.21504	0.21812	23.75	0.20969	0.21016
7.50	0.27321	0.28722	15.75	0.21347	0.21714	24.00	0.20960	0.21049
7.75	0.27867	0.28438	16.00	0.21144	0.21621	24.25	0.20985	0.21087
8.00	0.28154	0.28178	16.25	0.21005	0.21531	24.50	0.21032	0.21129
8.25	0.28382	0.27918	16.50	0.20983	0.21447	24.75	0.21100	0.21175
8.50	0.28351	0.27647	16.75	0.21032	0.21367	25.00	0.21198	0.21226
8.75	0.28014	0.27359	17.00	0.21168	0.21292	25.25	0.21299	0.21282
9.00	0.27437	0.27057	17.25	0.21334	0.21223	25.50	0.21395	0.21342
9.25	0.26974	0.26743	17.50	0.21447	0.21159	25.75	0.21493	0.21407
9.50	0.26707	0.26421	17.75	0.21539	0.21101	26.00	0.21568	0.21477
9.75	0.26489	0.26098	18.00	0.21553	0.21049	26.25	0.21642	0.21552
10.00	0.26248	0.25779	18.25	0.21488	0.21003	26.50	0.21694	0.21630
10.25	0.26100	0.25467	18.50	0.21370	0.20963	26.75	0.21755	0.21713
10.50	0.25662	0.25167	18.75	0.21176	0.20928	27.00	0.21814	0.21799
10.75	0.24912	0.24881	19.00	0.20969	0.20899	27.25	0.21868	0.21888
11.00	0.24061	0.24611	19.25	0.20776	0.20875	27.50	0.21939	0.21980
11.25	0.23339	0.24358	19.50	0.20655	0.20856	27.75	0.22023	0.22074
11.50	0.22879	0.24121	19.75	0.20588	0.20841	28.00	0.22089	0.22171
11.75	0.22698	0.23901	20.00	0.20586	0.20831	28.25	0.22191	0.22270
12.00	0.22766	0.23697	20.25	0.20617	0.20825	28.50	0.22299	0.22372
12.25	0.22968	0.23507	20.50	0.20656	0.20822	28.75	0.22421	0.22477
12.50	0.23325	0.23331	20.75	0.20713	0.20822	29.00	0.22550	0.22587
12.75	0.23672	0.23166	21.00	0.20763	0.20826	29.25	0.22705	0.22701
13.00	0.23904	0.23012	21.25	0.20803	0.20832	29.50	0.22838	0.22822
13.25	0.23962	0.22867	21.50	0.20847	0.20840	29.75	0.22987	0.22951
13.50	0.23777	0.22729	21.75	0.20904	0.20850	30.00	0.23141	0.23089
13.75	0.23394	0.22599	22.00	0.20961	0.20863	30.25	0.23311	0.23236
14.00	0.22940	0.22474	22.25	0.21002	0.20877	30.50	0.23462	0.23393
14.25	0.22508	0.22353	22.50	0.21018	0.20894	30.75	0.23604	0.23557
14.50	0.22167	0.22238	22.75	0.21018	0.20913	31.00	0.23750	0.23725
14.75	0.21912	0.22126	23.00	0.20995	0.20934	31.25	0.23887	0.23888
15.00	0.21743	0.22017	23.25	0.20990	0.20958	31.50	0.24025	0.24033
						31.75	0.24170	0.24140

Table S4. Equilibrium (r_e) and thermal–average (r_g, r_a) distances, vibrational corrections (see text for the notations), and mean amplitudes (u) for internuclear distances of the *meso* form of tetramezine obtained for 359 K at the GED(MP2) refinement (in Å).
(n - number of equivalent parameters)

Atomic pair	n	r_e	r_g	r_a	Δr	Δr(har)	Δr(kin)	Δr(dyn)	Δr(rot)	u
N6H8	2	1.0173	1.0388	1.0338	0.0215	0.0254	-0.0213	0.0174	0.0000	0.0732
C10H15	2	1.0789	1.1033	1.1025	0.0244	0.0650	-0.0569	0.0163	0.0000	0.0519
C9H11	2	1.0829	1.1069	1.1032	0.0240	0.0472	-0.0420	0.0188	0.0000	0.0662
C1H3	2	1.0839	1.1078	1.1033	0.0239	0.0361	-0.0312	0.0191	-0.0001	0.0721
C10H16	2	1.0843	1.1093	1.1081	0.0250	0.0654	-0.0574	0.0169	0.0001	0.0455
C9H13	2	1.0847	1.1078	1.1048	0.0231	0.0560	-0.0499	0.0170	0.0000	0.0605
C9H12	2	1.0852	1.1082	1.1052	0.0230	0.0545	-0.0485	0.0169	0.0001	0.0598
C10H14	2	1.0853	1.1105	1.1101	0.0252	0.0701	-0.0611	0.0163	-0.0001	0.0435
C1H4	2	1.0863	1.1095	1.1052	0.0232	0.0380	-0.0326	0.0179	-0.0001	0.0713
N5C7	2	1.4259	1.4356	1.4338	0.0097	0.0088	-0.0088	0.0096	0.0001	0.0505
N6C7	2	1.4389	1.4482	1.4465	0.0094	0.0116	-0.0098	0.0076	0.0000	0.0512
C1N5	2	1.4390	1.4512	1.4495	0.0122	0.0126	-0.0101	0.0098	-0.0001	0.0511
N5N6	2	1.5143	1.5264	1.5244	0.0122	0.0150	-0.0091	0.0063	0.0000	0.0578
C7C9	2	1.5181	1.5315	1.5300	0.0134	0.0198	-0.0180	0.0116	0.0000	0.0503
C7C10	2	1.5186	1.5319	1.5302	0.0132	0.0129	-0.0112	0.0116	-0.0001	0.0506
C1C2	1	1.5300	1.5424	1.5412	0.0124	0.0217	-0.0199	0.0106	0.0000	0.0433
H15H16	2	1.7571	1.7874	1.7876	0.0303	0.1102	-0.1018	0.0218	0.0001	0.0601
H14H16	2	1.7607	1.7951	1.7946	0.0343	0.1122	-0.1049	0.0271	-0.0001	0.0676
H12H13	2	1.7640	1.7939	1.7890	0.0299	0.0885	-0.0854	0.0267	0.0001	0.0979
H11H13	2	1.7652	1.7966	1.7915	0.0314	0.0811	-0.0784	0.0287	0.0000	0.0970
H3H4	2	1.7694	1.7969	1.7898	0.0275	0.0555	-0.0508	0.0228	0.0000	0.1141
H14H15	2	1.7723	1.8040	1.8042	0.0317	0.1094	-0.1011	0.0235	-0.0001	0.0618
H11H12	2	1.7772	1.8061	1.8009	0.0289	0.0778	-0.0752	0.0263	0.0000	0.0970
C7H8	2	2.0012	2.0200	2.0149	0.0188	0.0215	-0.0390	0.0363	0.0000	0.1024
N5H8	2	2.0119	2.0320	2.0266	0.0201	0.0270	-0.0535	0.0465	0.0001	0.1064
H4N5	2	2.0559	2.0782	2.0730	0.0223	0.0334	-0.0334	0.0223	0.0000	0.1060
H3H15	2	2.0835	2.2076	2.1825	0.1241	0.0545	0.0289	0.0408	-0.0001	0.2382
H3N5	2	2.1200	2.1428	2.1383	0.0228	0.0315	-0.0322	0.0234	0.0001	0.1001
C7H16	2	2.1284	2.1541	2.1489	0.0257	0.0381	-0.0386	0.0261	0.0001	0.1065
C7H11	2	2.1341	2.1609	2.1560	0.0268	0.0414	-0.0435	0.0290	-0.0001	0.1075
C7H14	2	2.1439	2.1667	2.1624	0.0228	0.0500	-0.0501	0.0230	-0.0001	0.1001
C7H13	2	2.1442	2.1653	2.1607	0.0212	0.0470	-0.0472	0.0214	0.0000	0.1036
C7H12	2	2.1465	2.1688	2.1642	0.0223	0.0480	-0.0500	0.0243	0.0000	0.1044
C1H17	2	2.1474	2.1735	2.1693	0.0262	0.0444	-0.0455	0.0273	0.0000	0.0960
C1H18	2	2.1507	2.1743	2.1699	0.0235	0.0443	-0.0463	0.0255	0.0000	0.0972
C7H15	2	2.1602	2.1855	2.1810	0.0254	0.0442	-0.0465	0.0277	0.0000	0.1061
H8H11	2	2.3402	2.3531	2.3310	0.0129	0.0391	-0.0386	0.0124	0.0000	0.2296
C1N19	2	2.3880	2.4066	2.4044	0.0186	0.0161	-0.0158	0.0183	0.0000	0.0730
C1N6	2	2.4166	2.4411	2.4389	0.0245	0.0198	-0.0264	0.0310	0.0001	0.0745
C1C7	2	2.4560	2.4742	2.4724	0.0182	0.0152	-0.0221	0.0251	0.0000	0.0683
H3H18	2	2.4738	2.5114	2.4997	0.0376	0.0574	-0.0591	0.0393	0.0000	0.1660
N5C9	2	2.4792	2.4936	2.4918	0.0145	0.0214	-0.0243	0.0173	0.0001	0.0697
H12H16	2	2.4832	2.5318	2.5065	0.0486	0.0671	-0.0151	-0.0034	0.0000	0.2568
H3N6	2	2.4935	2.5225	2.5118	0.0290	0.0344	-0.0349	0.0295	0.0000	0.1629
C9C10	2	2.5062	2.5235	2.5216	0.0173	0.0275	-0.0247	0.0144	0.0001	0.0739
N6C10	2	2.5248	2.5395	2.5375	0.0147	0.0150	-0.0179	0.0176	0.0000	0.0719
H8C9	2	2.5323	2.5575	2.5486	0.0252	0.0227	-0.0434	0.0460	-0.0001	0.1503
N5H11	2	2.5518	2.6064	2.5961	0.0546	0.0395	-0.0342	0.0493	0.0000	0.1657
N6C9	2	2.5552	2.5741	2.5723	0.0190	0.0225	-0.0246	0.0211	0.0000	0.0717
H13H14	2	2.5763	2.6527	2.6240	0.0764	0.0686	0.0054	0.0024	0.0000	0.2752
N5C10	2	2.5910	2.6085	2.6067	0.0175	0.0116	-0.0154	0.0213	0.0000	0.0685
H3N19	2	2.5930	2.6245	2.6136	0.0315	0.0370	-0.0329	0.0275	-0.0001	0.1512
N6H15	2	2.6409	2.6865	2.6750	0.0456	0.0354	-0.0343	0.0445	0.0000	0.1738

H3C7	2	2.6472	2.6955	2.6878	0.0482	0.0337	-0.0383	0.0528	0.0000	0.1457
H4N19	2	2.6479	2.6752	2.6636	0.0274	0.0342	-0.0333	0.0265	0.0000	0.1413
C9H16	2	2.6530	2.7041	2.6918	0.0511	0.0407	-0.0420	0.0524	0.0000	0.1849
H3C10	2	2.6687	2.7435	2.7292	0.0748	0.0300	-0.0305	0.0753	0.0000	0.1982
C10H13	2	2.7114	2.7693	2.7578	0.0579	0.0459	-0.0396	0.0516	0.0000	0.1819
N6H11	2	2.7228	2.7390	2.7307	0.0162	0.0396	-0.0310	0.0076	0.0000	0.1569
C1H15	2	2.7334	2.7797	2.7639	0.0463	0.0267	0.0079	0.0116	0.0001	0.2100
C10H12	2	2.7790	2.7724	2.7622	-0.0066	0.0506	-0.0398	-0.0174	0.0000	0.1722
C9H14	2	2.8075	2.8196	2.8050	0.0121	0.0498	-0.0246	-0.0130	-0.0001	0.2031
N5H15	2	2.8412	2.8723	2.8642	0.0310	0.0323	-0.0151	0.0139	-0.0001	0.1557
H8H12	2	2.8646	2.9421	2.9157	0.0775	0.0319	-0.0534	0.0990	0.0000	0.2747
H4C7	2	2.9066	2.9043	2.8960	-0.0023	0.0294	-0.0314	-0.0003	0.0000	0.1560
H13H16	2	2.9073	3.0105	2.9719	0.1032	0.0497	-0.0821	0.1357	-0.0001	0.3406
H4N20	2	2.9200	3.0224	2.9963	0.1024	0.0411	-0.0418	0.1031	0.0000	0.2584
C1C10	2	2.9420	2.9673	2.9634	0.0253	0.0120	-0.0248	0.0381	0.0000	0.1073
N6H12	2	2.9688	3.0235	3.0117	0.0548	0.0376	-0.0502	0.0673	0.0001	0.1891
N5H13	2	2.9791	2.9630	2.9524	-0.0161	0.0380	-0.0426	-0.0115	0.0000	0.1767
N5H14	2	2.9869	3.0213	3.0104	0.0344	0.0347	-0.0559	0.0555	0.0001	0.1803
H4H14	2	3.0064	3.0251	2.9702	0.0187	0.0309	-0.0410	0.0287	0.0001	0.3985
N6H16	2	3.0240	3.0313	3.0184	0.0073	0.0269	-0.0202	0.0007	-0.0001	0.1950
H3H17	1	3.0382	3.0694	3.0658	0.0311	0.0609	-0.0766	0.0468	0.0000	0.1049
H4H18	1	3.0447	3.0712	3.0678	0.0265	0.0616	-0.0787	0.0435	0.0001	0.1032
H3H14	2	3.0609	3.1447	3.0949	0.0838	0.0380	-0.0912	0.1371	-0.0001	0.3780
H4H15	2	3.0693	3.0463	2.9982	-0.0230	0.0255	0.0051	-0.0536	0.0000	0.3699
H4C10	2	3.1542	3.1367	3.1155	-0.0176	0.0195	-0.0244	-0.0127	0.0000	0.2530
C1H8	2	3.1687	3.1973	3.1938	0.0286	0.0313	-0.0622	0.0595	0.0000	0.1085
C1H14	2	3.1774	3.2199	3.1916	0.0424	0.0252	-0.0688	0.0861	-0.0001	0.2957
C1N20	2	3.1791	3.2416	3.2330	0.0625	0.0188	-0.0361	0.0798	0.0000	0.1666
H12H14	2	3.2338	3.1792	3.1424	-0.0546	0.0619	-0.0438	-0.0726	-0.0001	0.3340
H4H22	2	3.2859	3.3844	3.3565	0.0985	0.0511	-0.0521	0.0996	-0.0001	0.2652
H4N6	2	3.2993	3.3092	3.3058	0.0100	0.0327	-0.0488	0.0260	0.0001	0.1118
H8C10	2	3.3155	3.3379	3.3346	0.0223	0.0251	-0.0397	0.0369	0.0000	0.1056
N5H12	2	3.3449	3.3715	3.3678	0.0266	0.0417	-0.0640	0.0488	0.0001	0.1146
N6H14	2	3.3766	3.3903	3.3871	0.0137	0.0431	-0.0729	0.0435	0.0000	0.1066
H3H8	2	3.4313	3.4570	3.4480	0.0257	0.0418	-0.0645	0.0484	0.0000	0.1767
N6H13	2	3.4325	3.4383	3.4357	0.0058	0.0434	-0.0607	0.0232	-0.0001	0.1015
C10H11	2	3.4362	3.4573	3.4546	0.0211	0.0419	-0.0593	0.0385	0.0000	0.1021
N5H16	2	3.4449	3.4557	3.4526	0.0109	0.0301	-0.0504	0.0312	0.0000	0.1052
C9H15	2	3.4461	3.4603	3.4581	0.0142	0.0513	-0.0755	0.0384	0.0000	0.1002
H8H13	2	3.5373	3.5377	3.5305	0.0003	0.0438	-0.0904	0.0470	-0.0001	0.1621
H8H15	2	3.5959	3.6420	3.6325	0.0461	0.0429	-0.0604	0.0636	0.0000	0.1853
H3N20	2	3.6296	3.6908	3.6725	0.0612	0.0266	-0.0531	0.0877	0.0000	0.2379
H3H16	2	3.6333	3.6766	3.6638	0.0433	0.0453	-0.0650	0.0629	0.0001	0.2183
N5N19	1	3.6339	3.6476	3.6461	0.0136	0.0067	-0.0205	0.0274	0.0000	0.0724
H8H16	2	3.6539	3.6762	3.6639	0.0224	0.0315	-0.0241	0.0149	0.0001	0.2110
C1H22	2	3.6656	3.7301	3.7195	0.0645	0.0290	-0.0616	0.0971	0.0000	0.1982
H11H16	2	3.6737	3.6979	3.6897	0.0241	0.0483	-0.0748	0.0506	0.0000	0.1776
C1C21	2	3.6934	3.7185	3.7166	0.0251	0.0120	-0.0328	0.0459	0.0000	0.0825
H12H15	2	3.7129	3.7137	3.7046	0.0008	0.0676	-0.1011	0.0343	0.0000	0.1886
H13H15	2	3.7427	3.7721	3.7645	0.0294	0.0635	-0.0870	0.0529	0.0000	0.1807
C1C9	2	3.7492	3.7676	3.7661	0.0184	0.0272	-0.0345	0.0257	0.0000	0.0791
H11H14	2	3.7506	3.7840	3.7732	0.0334	0.0582	-0.0659	0.0411	0.0000	0.2026
H4C21	2	3.8326	3.8847	3.8743	0.0520	0.0255	-0.0493	0.0758	0.0000	0.1790
H3H22	2	3.8921	3.9631	3.9369	0.0709	0.0354	-0.0778	0.1134	-0.0001	0.2943
C1H11	2	3.9615	4.0179	4.0107	0.0564	0.0403	-0.0451	0.0612	0.0000	0.1721
C1H16	2	3.9692	3.9737	3.9698	0.0045	0.0302	-0.0689	0.0432	0.0000	0.1255
H4C9	2	4.0004	4.0022	3.9953	0.0018	0.0385	-0.0357	-0.0010	0.0000	0.1664
H3C21	2	4.0137	4.0312	4.0242	0.0175	0.0226	-0.0437	0.0385	0.0001	0.1515
H4H13	2	4.0158	3.9955	3.9767	-0.0203	0.0491	-0.0197	-0.0497	0.0000	0.2701
H4H8	2	4.0181	4.0392	4.0351	0.0211	0.0412	-0.0886	0.0685	0.0000	0.1342

C1H13	2	4.0571	4.0479	4.0385	-0.0092	0.0383	-0.0395	-0.0080	0.0000	0.1942
C1H29	2	4.1134	4.1781	4.1681	0.0647	0.0193	-0.0135	0.0589	0.0000	0.2062
H8H14	2	4.1227	4.1386	4.1348	0.0159	0.0481	-0.0919	0.0598	-0.0001	0.1308
H3C9	2	4.1237	4.1704	4.1656	0.0467	0.0416	-0.0562	0.0613	0.0000	0.1459
H4H16	2	4.2352	4.1956	4.1797	-0.0396	0.0356	-0.0815	0.0064	-0.0001	0.2545
H11H15	2	4.2666	4.2879	4.2843	0.0213	0.0625	-0.0979	0.0566	0.0001	0.1368
H4H11	2	4.2772	4.3405	4.3279	0.0633	0.0496	-0.0548	0.0685	0.0000	0.2323
H4H29	2	4.2937	4.4041	4.3843	0.1104	0.0306	-0.0359	0.1157	0.0000	0.2929
N5N20	2	4.3687	4.4168	4.4100	0.0481	0.0082	-0.0427	0.0826	0.0000	0.1378
C1C24	2	4.4067	4.4350	4.4323	0.0283	0.0082	-0.0446	0.0646	0.0001	0.1100
H3H13	2	4.4897	4.5297	4.5193	0.0399	0.0519	-0.0671	0.0551	0.0000	0.2174
H3H11	2	4.5273	4.5854	4.5786	0.0581	0.0520	-0.0733	0.0794	0.0000	0.1823
C1H12	2	4.5771	4.5972	4.5948	0.0200	0.0438	-0.0737	0.0499	0.0000	0.1109
H3H25	2	4.6457	4.7125	4.6938	0.0669	0.0445	-0.0214	0.0438	0.0000	0.2759
H4C24	2	4.6465	4.7080	4.6978	0.0615	0.0188	-0.0639	0.1066	0.0000	0.2163
N5H29	2	4.6638	4.7386	4.7252	0.0748	0.0183	-0.0028	0.0593	0.0000	0.2454
C1H28	2	4.7049	4.7276	4.7087	0.0227	0.0155	-0.0870	0.0942	0.0000	0.2951
H3H12	2	4.7672	4.8173	4.8106	0.0501	0.0571	-0.0841	0.0771	0.0000	0.1846
C1H25	2	4.7896	4.8436	4.8353	0.0540	0.0319	-0.0316	0.0537	0.0000	0.2020
N5C21	2	4.8033	4.8235	4.8217	0.0201	0.0046	-0.0385	0.0540	0.0000	0.0895
H3H29	2	4.8472	4.8806	4.8706	0.0334	0.0216	-0.0403	0.0520	0.0001	0.2203
C1C23	2	4.8643	4.8772	4.8752	0.0129	0.0191	-0.0384	0.0322	0.0000	0.0986
H4H25	2	4.8789	4.9321	4.9154	0.0532	0.0399	-0.0411	0.0543	0.0001	0.2406
H4H12	2	4.9149	4.8928	4.8859	-0.0222	0.0522	-0.0770	0.0027	-0.0001	0.1866
H3C23	2	4.9151	4.9191	4.9101	0.0040	0.0289	-0.0377	0.0129	-0.0001	0.1909
H3C24	2	4.9393	4.9475	4.9427	0.0081	0.0143	-0.0585	0.0524	-0.0001	0.1486
N5H22	2	4.9862	5.0304	5.0223	0.0442	0.0130	-0.0676	0.0988	0.0000	0.1746
H4C23	2	5.0179	5.0527	5.0435	0.0348	0.0274	-0.0554	0.0628	0.0000	0.1714
H3H28	2	5.1292	5.1335	5.1140	0.0044	0.0219	-0.0878	0.0702	0.0001	0.3134
H4H28	2	5.1632	5.2021	5.1843	0.0390	0.0236	-0.1180	0.1333	0.0001	0.3010
N5C24	2	5.1762	5.2074	5.2027	0.0311	0.0056	-0.0486	0.0741	0.0000	0.1540
H3H27	2	5.2505	5.1767	5.1551	-0.0738	0.0331	-0.0379	-0.0690	0.0000	0.3221
C1H27	2	5.2745	5.2263	5.2161	-0.0482	0.0246	-0.0452	-0.0276	0.0000	0.2291
N5H28	2	5.3612	5.3925	5.3675	0.0313	0.0109	-0.0901	0.1105	0.0000	0.3596
C1H30	2	5.3822	5.3926	5.3886	0.0104	0.0215	-0.0813	0.0701	0.0001	0.1473
N6N20	1	5.4362	5.4998	5.4930	0.0636	0.0057	-0.0601	0.1180	0.0000	0.1951
H4H30	2	5.5001	5.5506	5.5365	0.0505	0.0306	-0.0855	0.1054	0.0000	0.2767
N6H29	2	5.5698	5.6531	5.6361	0.0833	0.0155	-0.0164	0.0842	0.0000	0.3012
N6C21	2	5.5864	5.6316	5.6268	0.0452	0.0052	-0.0554	0.0954	0.0000	0.1432
H4H27	2	5.6230	5.5916	5.5795	-0.0314	0.0298	-0.0754	0.0142	0.0000	0.2381
H8H29	2	5.7094	5.7950	5.7702	0.0856	0.0218	-0.0367	0.1005	0.0000	0.3632
C1H26	2	5.7096	5.7442	5.7407	0.0345	0.0318	-0.0820	0.0848	-0.0001	0.1421
H4H26	2	5.7322	5.8113	5.7980	0.0791	0.0397	-0.0927	0.1321	0.0000	0.2384
H3H26	2	5.8540	5.8752	5.8664	0.0212	0.0380	-0.0864	0.0696	0.0000	0.2113
N6H28	2	5.8683	5.9435	5.9170	0.0752	0.0152	-0.0904	0.1504	0.0000	0.3837
H3H30	2	5.9133	5.9053	5.9002	-0.0080	0.0246	-0.0974	0.0648	0.0000	0.1662
N6C24	2	5.9418	5.9983	5.9917	0.0565	0.0072	-0.0626	0.1119	0.0000	0.1971
N6H22	2	6.0040	6.0609	6.0526	0.0569	0.0086	-0.0915	0.1398	0.0000	0.2196
H8H28	2	6.0309	6.1095	6.0742	0.0786	0.0194	-0.1064	0.1656	0.0000	0.4474
C7H22	2	6.0667	6.1073	6.0997	0.0406	0.0081	-0.0807	0.1132	0.0000	0.2025
N5C23	2	6.0831	6.0863	6.0849	0.0033	0.0076	-0.0457	0.0413	0.0001	0.0923
C7C21	1	6.0831	6.1065	6.1051	0.0234	0.0027	-0.0527	0.0734	0.0000	0.0922
C7H29	2	6.0874	6.1593	6.1489	0.0718	0.0142	-0.0129	0.0706	-0.0001	0.2464
N5H25	2	6.1282	6.1683	6.1621	0.0401	0.0155	-0.0432	0.0678	0.0000	0.1943
H8C24	2	6.1821	6.2380	6.2258	0.0559	0.0118	-0.0858	0.1298	0.0001	0.2743
N5H30	2	6.1878	6.1909	6.1853	0.0031	0.0154	-0.0904	0.0780	0.0001	0.1795
N5H27	2	6.3904	6.3416	6.3324	-0.0488	0.0131	-0.0460	-0.0160	0.0001	0.2248
H11H29	2	6.5176	6.6406	6.6190	0.1230	0.0309	0.0129	0.0792	0.0000	0.3607
C7C24	2	6.5651	6.5992	6.5957	0.0341	0.0041	-0.0605	0.0905	0.0000	0.1503
H8H22	1	6.6794	6.7270	6.7193	0.0476	0.0091	-0.1221	0.1606	0.0000	0.2278

N6C23	2	6.6929	6.7161	6.7095	0.0232	0.0068	-0.0600	0.0764	0.0000	0.1158
N6H25	2	6.6952	6.7666	6.7525	0.0714	0.0120	-0.0588	0.1183	-0.0001	0.2263
C7H28	2	6.7058	6.7474	6.7275	0.0416	0.0092	-0.0993	0.1316	0.0001	0.3588
N6H27	2	6.7900	6.7611	6.7436	-0.0289	0.0128	-0.0498	0.0081	0.0000	0.2394
H15H29	1	6.8148	6.9022	6.8906	0.0874	0.0148	-0.0055	0.0781	0.0000	0.2834
N5H26	2	6.9134	6.9282	6.9259	0.0149	0.0182	-0.0887	0.0854	0.0000	0.1282
C9H29	2	6.9204	6.9878	6.9758	0.0673	0.0212	-0.0086	0.0547	0.0000	0.2742
C10H29	2	6.9972	7.0683	7.0611	0.0711	0.0103	-0.0302	0.0911	-0.0001	0.2253
N6H30	2	7.0131	7.0361	7.0300	0.0230	0.0142	-0.1138	0.1225	0.0001	0.2059
H14H29	2	7.1513	7.2360	7.2196	0.0847	0.0175	-0.0633	0.1305	0.0000	0.3417
C7H25	2	7.1702	7.2183	7.2110	0.0482	0.0104	-0.0533	0.0911	0.0000	0.2226
H13H29	2	7.2334	7.2331	7.2151	-0.0003	0.0266	-0.0106	-0.0163	0.0000	0.3458
H8C23	2	7.2417	7.2569	7.2477	0.0152	0.0061	-0.0826	0.0918	-0.0001	0.1782
H8H30	2	7.2463	7.2638	7.2523	0.0175	0.0165	-0.1401	0.1411	0.0000	0.2860
C10H25	2	7.2498	7.3181	7.3057	0.0683	0.0154	-0.0504	0.1032	0.0001	0.2973
C7C23	2	7.2626	7.2693	7.2675	0.0068	0.0045	-0.0597	0.0620	0.0000	0.1052
H8H27	2	7.2735	7.2455	7.2240	-0.0280	0.0115	-0.0648	0.0253	0.0000	0.2732
C10C24	1	7.3354	7.3753	7.3724	0.0399	0.0032	-0.0693	0.1060	0.0000	0.1446
H8H25	2	7.3684	7.4280	7.4135	0.0596	0.0098	-0.0858	0.1356	0.0000	0.2455
H11H28	2	7.3796	7.4481	7.4180	0.0685	0.0190	-0.0922	0.1418	-0.0001	0.4626
C10H28	2	7.5358	7.5812	7.5670	0.0455	0.0084	-0.1062	0.1433	0.0000	0.3254
C7H27	2	7.5508	7.5003	7.4910	-0.0505	0.0093	-0.0586	-0.0012	0.0000	0.2355
C9C24	2	7.5611	7.5831	7.5780	0.0220	0.0083	-0.0652	0.0790	-0.0001	0.1930
C7H30	2	7.5845	7.5873	7.5831	0.0028	0.0114	-0.1020	0.0934	0.0000	0.1728
N6H26	2	7.6382	7.6564	7.6513	0.0182	0.0155	-0.1053	0.1080	0.0000	0.1472
C9H28	2	7.7283	7.7588	7.7377	0.0305	0.0117	-0.1093	0.1281	0.0000	0.3966
H12H29	2	7.8622	7.9431	7.9303	0.0809	0.0289	-0.0552	0.1072	0.0000	0.3083
H14H28	1	7.8819	7.9182	7.8957	0.0363	0.0120	-0.1555	0.1798	0.0000	0.4195
C10H27	2	7.9159	7.8694	7.8581	-0.0465	0.0126	-0.0670	0.0079	0.0000	0.2882
H15H30	2	7.9804	8.0274	8.0196	0.0470	0.0179	-0.0671	0.0963	-0.0001	0.2477
C7H26	2	8.1409	8.1580	8.1557	0.0171	0.0132	-0.1036	0.1075	0.0000	0.1406
H8H26	2	8.1536	8.1561	8.1488	0.0025	0.0134	-0.1282	0.1173	0.0000	0.2073
H11H30	2	8.2170	8.2486	8.2342	0.0316	0.0181	-0.0895	0.1030	0.0000	0.3265
H13H28	2	8.2179	8.1729	8.1492	-0.0451	0.0150	-0.1229	0.0628	0.0000	0.4354
C10H30	2	8.3235	8.3371	8.3336	0.0136	0.0108	-0.1066	0.1095	-0.0001	0.1724
H14H30	2	8.4566	8.4817	8.4665	0.0251	0.0159	-0.1329	0.1421	0.0000	0.3538
C10H26	2	8.4594	8.5006	8.4945	0.0413	0.0168	-0.1104	0.1349	0.0000	0.2279
C9H25	2	8.5345	8.5571	8.5519	0.0226	0.0055	-0.0668	0.0839	0.0000	0.2110
H12H28	2	8.5431	8.6086	8.5865	0.0656	0.0204	-0.1477	0.1929	0.0000	0.4239
C9H30	2	8.5476	8.5323	8.5255	-0.0153	0.0126	-0.1035	0.0756	0.0000	0.2228
C9C23	1	8.5495	8.5384	8.5370	-0.0111	0.0020	-0.0704	0.0572	0.0001	0.1091
H11H25	1	8.6560	8.7054	8.6978	0.0494	0.0085	-0.0728	0.1136	0.0001	0.2563
H11H27	2	8.8010	8.7760	8.7648	-0.0250	0.0097	-0.0636	0.0289	0.0000	0.2887
H13H30	2	8.8436	8.7605	8.7464	-0.0832	0.0164	-0.0950	-0.0045	-0.0001	0.3227
C9H27	2	8.8589	8.7984	8.7910	-0.0605	0.0061	-0.0711	0.0045	0.0000	0.2330
H13H27	1	9.2855	9.1726	9.1626	-0.1128	0.0099	-0.0826	-0.0401	0.0000	0.3016
H11H26	2	9.3105	9.3407	9.3341	0.0302	0.0112	-0.1044	0.1234	0.0000	0.2389
H16H30	1	9.3330	9.3158	9.3119	-0.0173	0.0160	-0.1491	0.1159	-0.0001	0.1880
C9H26	2	9.3675	9.3647	9.3621	-0.0028	0.0088	-0.1109	0.0993	0.0000	0.1424
H12H30	2	9.4745	9.4730	9.4661	-0.0015	0.0191	-0.1529	0.1323	0.0000	0.2468
H12H27	2	9.6113	9.5661	9.5562	-0.0452	0.0123	-0.1065	0.0490	0.0000	0.2587
H12H26	1	10.2352	10.2322	10.2295	-0.0030	0.0139	-0.1544	0.1376	-0.0001	0.1681

Table S5. Equilibrium (r_e) and thermal–average (r_g, r_a) distances, vibrational corrections (see text for the notations) and mean amplitudes (u) for internuclear distances for *enantiomeric* forms of tetramezine obtained for 359 K at the GED(MP2) refinement (in Å).
(n - number of equivalent parameters)

Atomic pair	n	r_e	r_g	r_a	Δr	Δr(harm)	Δr(kin)	Δr(dyn)	Δr(rot)	u
N6H8	2	1.0173	1.0417	1.0366	0.0244	0.0326	-0.0218	0.0136	0.0000	0.0743
C10H15	2	1.0790	1.1188	1.1118	0.0399	0.0681	-0.0559	0.0277	0.0000	0.0914
C9H11	2	1.0829	1.1089	1.1078	0.0260	0.0692	-0.0563	0.0132	-0.0001	0.0659
C10H16	2	1.0844	1.1194	1.1152	0.0350	0.0657	-0.0590	0.0283	0.0000	0.0702
C9H13	2	1.0847	1.1098	1.1098	0.0251	0.0734	-0.0589	0.0106	0.0000	0.0590
C9H12	2	1.0853	1.1086	1.1064	0.0234	0.0593	-0.0499	0.0140	0.0000	0.0594
C10H14	2	1.0853	1.1261	1.1205	0.0408	0.0824	-0.0697	0.0281	0.0000	0.0856
C1H3	2	1.0855	1.1129	1.1075	0.0273	0.0238	-0.0182	0.0217	0.0000	0.0773
C1H4	2	1.0864	1.1099	1.1047	0.0235	0.0271	-0.0203	0.0167	0.0000	0.0765
N5C7	2	1.4258	1.4288	1.4274	0.0030	0.0163	-0.0125	-0.0008	0.0000	0.0491
C1N5	2	1.4387	1.4544	1.4525	0.0157	0.0128	-0.0093	0.0122	0.0000	0.0522
N6C7	2	1.4392	1.4506	1.4498	0.0114	0.0295	-0.0211	0.0030	0.0000	0.0515
N5N6	2	1.5142	1.5270	1.5251	0.0128	0.0259	-0.0156	0.0025	0.0000	0.0574
C7C9	2	1.5182	1.5308	1.5295	0.0125	0.0241	-0.0206	0.0090	0.0000	0.0495
C7C10	2	1.5192	1.5320	1.5315	0.0128	0.0377	-0.0286	0.0038	-0.0001	0.0506
C1C2	1	1.5300	1.5423	1.5407	0.0122	0.0117	-0.0097	0.0103	-0.0001	0.0509
H15H16	2	1.7558	1.8117	1.8001	0.0559	0.1004	-0.0953	0.0509	-0.0001	0.1446
H14H16	2	1.7606	1.8213	1.8120	0.0608	0.1197	-0.1096	0.0507	0.0000	0.1342
H12H13	2	1.7642	1.7971	1.7952	0.0329	0.1070	-0.0937	0.0197	-0.0001	0.0950
H11H13	2	1.7651	1.7954	1.7947	0.0304	0.1131	-0.0964	0.0137	0.0000	0.0971
H3H4	2	1.7699	1.8034	1.7949	0.0336	0.0343	-0.0282	0.0275	0.0000	0.1241
H14H15	2	1.7723	1.8278	1.8178	0.0555	0.1266	-0.1112	0.0401	0.0000	0.1416
H11H12	2	1.7780	1.8077	1.8067	0.0297	0.1069	-0.0924	0.0152	0.0000	0.0964
C7H8	2	2.0018	2.0257	2.0216	0.0239	0.0470	-0.0507	0.0275	0.0001	0.1006
N5H8	2	2.0101	2.0306	2.0258	0.0204	0.0342	-0.0567	0.0429	0.0000	0.1005
H4N5	2	2.0572	2.0790	2.0732	0.0218	0.0280	-0.0303	0.0242	-0.0001	0.1106
H3H15	2	2.0726	2.3710	2.3417	0.2984	0.0741	-0.0061	0.2305	-0.0001	0.2591
H3N5	2	2.1105	2.1495	2.1448	0.0390	0.0228	-0.0166	0.0328	0.0000	0.0994
C7H16	2	2.1286	2.1570	2.1543	0.0284	0.0680	-0.0666	0.0271	-0.0001	0.1017
C7H11	2	2.1330	2.1598	2.1565	0.0268	0.0633	-0.0588	0.0223	0.0000	0.1026
C1H17	2	2.1440	2.1751	2.1699	0.0311	0.0231	-0.0310	0.0390	0.0000	0.1040
C7H13	2	2.1443	2.1678	2.1655	0.0236	0.0677	-0.0603	0.0162	0.0000	0.0959
C7H14	2	2.1447	2.1839	2.1788	0.0392	0.0819	-0.0688	0.0262	-0.0001	0.1176
C7H12	2	2.1472	2.1728	2.1669	0.0255	0.0404	-0.0433	0.0284	0.0000	0.1130
C1H18	2	2.1491	2.1668	2.1613	0.0176	0.0243	-0.0246	0.0179	0.0000	0.1094
C7H15	2	2.1626	2.1906	2.1860	0.0280	0.0736	-0.0605	0.0149	0.0000	0.1091
H8H11	2	2.3413	2.3751	2.3529	0.0337	0.0659	-0.0363	0.0042	-0.0001	0.2388
H3H17	1	2.3899	2.4803	2.4672	0.0905	0.0325	-0.0232	0.0811	0.0001	0.1777
C1N19	2	2.4085	2.4204	2.4182	0.0119	0.0156	-0.0068	0.0031	0.0000	0.0723
C1N6	2	2.4111	2.4608	2.4583	0.0497	0.0182	-0.0188	0.0503	0.0000	0.0776
C1C7	2	2.4544	2.4812	2.4793	0.0268	0.0103	-0.0153	0.0318	0.0000	0.0697
H3N6	2	2.4762	2.5450	2.5327	0.0688	0.0228	0.0186	0.0274	0.0000	0.1521
N5C9	2	2.4773	2.4795	2.4781	0.0022	0.0200	-0.0223	0.0045	0.0000	0.0638
H12H16	2	2.4795	2.4862	2.4612	0.0066	0.0933	-0.0369	-0.0498	0.0000	0.2597
C9C10	2	2.5049	2.5355	2.5341	0.0305	0.0520	-0.0417	0.0202	0.0000	0.0756
N6C10	2	2.5259	2.5410	2.5406	0.0151	0.0525	-0.0457	0.0083	0.0000	0.0725
H8C9	2	2.5326	2.5563	2.5494	0.0237	0.0518	-0.0569	0.0287	0.0001	0.1495
H3H18	2	2.5337	2.5172	2.5045	-0.0164	0.0330	-0.0704	0.0210	0.0000	0.1704
N5H11	2	2.5459	2.5760	2.5675	0.0301	0.0412	-0.0428	0.0317	0.0000	0.1498
N6C9	2	2.5553	2.5718	2.5710	0.0165	0.0420	-0.0359	0.0104	0.0000	0.0735
H13H14	2	2.5763	2.8330	2.8009	0.2567	0.0837	0.0048	0.1682	0.0000	0.2981
H4N19	2	2.5893	2.6619	2.6489	0.0726	0.0227	0.0245	0.0253	0.0001	0.1723
N5C10	2	2.5955	2.5963	2.5961	0.0007	0.0492	-0.0382	-0.0103	0.0000	0.0696

H3C7	2	2.6246	2.7218	2.7132	0.0972	0.0182	-0.0398	0.1189	-0.0001	0.1438
N6H15	2	2.6440	2.6172	2.6112	-0.0268	0.0815	-0.0700	-0.0384	0.0001	0.1410
H3C10	2	2.6488	2.7660	2.7467	0.1173	0.0343	-0.0820	0.1650	0.0000	0.1831
C9H16	2	2.6488	2.5996	2.5923	-0.0492	0.0871	-0.0957	-0.0407	0.0001	0.1600
C10H13	2	2.7093	2.7620	2.7485	0.0527	0.0748	-0.0726	0.0505	0.0000	0.1889
N6H11	2	2.7226	2.7499	2.7417	0.0274	0.0645	-0.0364	-0.0007	0.0000	0.1675
C1H15	2	2.7462	2.9468	2.9263	0.2007	0.0536	0.0241	0.1229	0.0001	0.2448
C10H12	2	2.7783	2.8229	2.8113	0.0446	0.0542	-0.0288	0.0192	0.0000	0.1812
C9H14	2	2.8082	2.9850	2.9664	0.1768	0.0691	-0.0195	0.1272	0.0000	0.2352
N5N19	1	2.8483	2.7639	2.7572	-0.0844	0.0259	-0.0520	-0.0584	0.0001	0.1434
N5H15	2	2.8516	2.9446	2.9333	0.0930	0.0778	-0.0273	0.0425	0.0000	0.1865
H8H12	2	2.8629	2.9065	2.8800	0.0436	0.0532	-0.0823	0.0726	0.0001	0.2772
H4N20	2	2.8714	3.0594	3.0387	0.1880	0.0344	-0.0970	0.2505	0.0001	0.2331
H13H16	2	2.9011	2.7822	2.7345	-0.1189	0.0995	-0.1680	-0.0503	-0.0001	0.3508
H4C7	2	2.9121	2.8964	2.8887	-0.0157	0.0203	0.0187	-0.0547	0.0000	0.1333
C1C10	2	2.9480	2.9657	2.9621	0.0177	0.0296	-0.0304	0.0185	0.0000	0.1125
N6H12	2	2.9679	3.0039	2.9918	0.0360	0.0449	-0.0651	0.0562	0.0000	0.1930
N5H13	2	2.9792	2.9735	2.9663	-0.0056	0.0543	-0.0382	-0.0218	0.0001	0.1688
N5H14	2	2.9913	2.9070	2.9007	-0.0844	0.0880	-0.0959	-0.0764	-0.0001	0.1582
H4H14	2	3.0246	2.7429	2.6808	-0.2817	0.0660	0.0021	-0.3498	0.0000	0.3767
N6H16	2	3.0254	3.1593	3.1451	0.1339	0.0605	-0.0403	0.1138	-0.0001	0.2221
H4H18	1	3.0377	3.0629	3.0576	0.0252	0.0302	-0.0398	0.0348	0.0000	0.1282
H3H14	2	3.0420	2.9154	2.8541	-0.1266	0.0632	-0.2144	0.0245	0.0001	0.3442
H4H15	2	3.0896	3.2715	3.2192	0.1819	0.0396	0.1338	0.0085	0.0000	0.3237
C1H8	2	3.1626	3.2095	3.2060	0.0468	0.0310	-0.0559	0.0717	0.0000	0.1074
H4C10	2	3.1697	3.1163	3.0975	-0.0534	0.0308	0.0590	-0.1431	-0.0001	0.1897
C1N20	2	3.1808	3.2927	3.2857	0.1118	0.0176	-0.0851	0.1794	-0.0001	0.1278
C1H14	2	3.1846	2.9855	2.9557	-0.1991	0.0631	-0.1144	-0.1479	0.0001	0.2942
H4H22	2	3.2059	3.4089	3.3864	0.2030	0.0491	-0.0637	0.2176	0.0000	0.2822
H12H14	2	3.2358	3.4516	3.4145	0.2158	0.0634	-0.0008	0.1532	0.0000	0.3502
H4N6	2	3.2984	3.3180	3.3133	0.0196	0.0256	-0.0172	0.0111	0.0001	0.1055
H8C10	2	3.3159	3.3466	3.3450	0.0307	0.0719	-0.0680	0.0268	0.0000	0.1072
H3N19	2	3.3393	3.3716	3.3684	0.0322	0.0189	-0.0261	0.0394	0.0000	0.1037
N5H12	2	3.3430	3.3512	3.3477	0.0082	0.0362	-0.0641	0.0362	-0.0001	0.1087
N6H14	2	3.3776	3.3513	3.3517	-0.0262	0.0946	-0.1122	-0.0087	0.0001	0.0843
H3H8	2	3.4161	3.4735	3.4616	0.0574	0.0326	-0.0064	0.0312	0.0000	0.1637
N6H13	2	3.4331	3.4445	3.4449	0.0114	0.0808	-0.0802	0.0109	-0.0001	0.0980
C10H11	2	3.4346	3.4626	3.4619	0.0280	0.0877	-0.0929	0.0332	0.0000	0.0988
C9H15	2	3.4460	3.4588	3.4572	0.0127	0.0807	-0.0927	0.0247	0.0000	0.0967
N5H16	2	3.4477	3.4725	3.4710	0.0248	0.0662	-0.0771	0.0357	0.0000	0.1097
H8H13	2	3.5385	3.5480	3.5448	0.0096	0.0895	-0.1076	0.0277	0.0000	0.1632
H8H15	2	3.5981	3.5654	3.5598	-0.0326	0.0955	-0.0976	-0.0305	0.0000	0.1595
H3H16	2	3.6147	3.8247	3.8040	0.2099	0.0453	-0.0900	0.2547	-0.0001	0.2421
H8H16	2	3.6535	3.7854	3.7743	0.1319	0.0808	-0.0533	0.1044	0.0000	0.2270
H11H16	2	3.6702	3.6312	3.6269	-0.0390	0.1109	-0.1340	-0.0160	0.0001	0.1740
C1H22	2	3.6741	3.7729	3.7652	0.0987	0.0319	-0.1033	0.1701	0.0000	0.1697
C1C21	2	3.7039	3.7362	3.7343	0.0323	0.0085	-0.0420	0.0659	-0.0001	0.0777
H12H15	2	3.7112	3.6715	3.6645	-0.0397	0.0782	-0.1056	-0.0123	0.0000	0.1721
H13H15	2	3.7423	3.8186	3.8078	0.0763	0.0959	-0.1104	0.0908	0.0000	0.2040
C1C9	2	3.7482	3.7618	3.7603	0.0135	0.0209	-0.0291	0.0218	-0.0001	0.0758
H11H14	2	3.7500	3.8873	3.8761	0.1373	0.1019	-0.0902	0.1256	0.0000	0.2115
H4C21	2	3.7878	3.8879	3.8781	0.1000	0.0154	-0.0570	0.1417	-0.0001	0.1875
N5N20	2	3.9499	3.9092	3.8944	-0.0408	0.0144	-0.1645	0.1093	0.0000	0.1509
C1H11	2	3.9561	3.9849	3.9789	0.0288	0.0408	-0.0559	0.0438	0.0001	0.1562
C1H16	2	3.9745	4.0395	4.0349	0.0649	0.0446	-0.0690	0.0893	0.0000	0.1453
H4C9	2	4.0072	3.9801	3.9742	-0.0271	0.0303	-0.0058	-0.0516	0.0000	0.1560
H4H8	2	4.0160	4.0428	4.0383	0.0267	0.0371	-0.0774	0.0670	0.0000	0.1347
H3N20	2	4.0167	4.1962	4.1873	0.1794	0.0169	-0.0563	0.2188	0.0000	0.1878
H4H13	2	4.0268	3.9902	3.9760	-0.0367	0.0559	0.0135	-0.1061	0.0000	0.2551
C1H13	2	4.0595	4.0572	4.0500	-0.0023	0.0460	-0.0348	-0.0135	0.0000	0.1825

H3C9	2	4.1022	4.1903	4.1842	0.0881	0.0262	-0.0636	0.1255	0.0000	0.1458
C1H29	2	4.1137	4.3362	4.3247	0.2224	0.0344	-0.0456	0.2336	0.0000	0.2275
H8H14	2	4.1238	4.1497	4.1473	0.0259	0.1051	-0.1243	0.0452	-0.0001	0.1338
N5H22	2	4.1864	4.1112	4.0884	-0.0752	0.0306	-0.2315	0.1256	0.0001	0.2145
H4H16	2	4.2502	4.1774	4.1665	-0.0728	0.0473	-0.0034	-0.1167	0.0000	0.1870
H11H15	2	4.2671	4.2871	4.2852	0.0200	0.1127	-0.1283	0.0356	0.0000	0.1343
N5C21	2	4.2672	4.1559	4.1513	-0.1114	0.0113	-0.0513	-0.0713	-0.0001	0.1425
H4H11	2	4.2768	4.2842	4.2727	0.0073	0.0487	-0.0742	0.0329	-0.0001	0.2201
H4H29	2	4.3259	4.4819	4.4624	0.1560	0.0416	-0.1564	0.2708	0.0000	0.2326
C1C24	2	4.4112	4.4376	4.4344	0.0263	0.0166	-0.0725	0.0822	0.0000	0.1105
H3H29	2	4.4619	4.7965	4.7801	0.3346	0.0365	-0.0272	0.3253	0.0000	0.2834
H3H13	2	4.4696	4.5568	4.5448	0.0872	0.0481	-0.1032	0.1423	0.0000	0.1995
H3H11	2	4.5066	4.5821	4.5756	0.0755	0.0445	-0.0763	0.1074	-0.0001	0.1752
H3C21	2	4.5144	4.5936	4.5900	0.0792	0.0112	-0.0524	0.1205	-0.0001	0.1231
C1H12	2	4.5761	4.6007	4.5976	0.0246	0.0307	-0.0622	0.0561	0.0000	0.1181
H3H22	2	4.6192	4.7728	4.7632	0.1536	0.0257	-0.0731	0.2009	0.0001	0.2125
H4C24	2	4.6438	4.7092	4.6980	0.0654	0.0209	-0.1388	0.1833	0.0000	0.1734
C1H28	2	4.7137	4.4497	4.4294	-0.2640	0.0370	-0.1229	-0.1781	0.0000	0.2991
H3H12	2	4.7446	4.8537	4.8449	0.1091	0.0340	-0.0780	0.1531	0.0000	0.1975
H4H25	2	4.7836	4.8906	4.8720	0.1070	0.0363	0.0419	0.0288	0.0000	0.2716
N5H25	2	4.8051	4.6170	4.6002	-0.1880	0.0513	-0.0602	-0.1792	0.0001	0.2858
C1H25	2	4.8126	4.8078	4.8003	-0.0048	0.0364	-0.0223	-0.0189	0.0000	0.1860
C1C23	2	4.8843	4.8766	4.8751	-0.0077	0.0169	-0.0261	0.0015	0.0000	0.0893
H4H12	2	4.9231	4.8856	4.8790	-0.0376	0.0374	-0.0253	-0.0497	0.0000	0.1745
H4C23	2	4.9472	5.0339	5.0250	0.0868	0.0188	-0.0124	0.0804	0.0000	0.2089
H3C24	2	4.9523	5.0418	5.0351	0.0896	0.0195	-0.0821	0.1522	0.0000	0.1723
N5C23	2	5.1069	4.9211	4.9137	-0.1858	0.0246	-0.0313	-0.1791	0.0000	0.1930
N5H29	2	5.1385	5.2821	5.2716	0.1436	0.0194	-0.0039	0.1281	0.0000	0.2308
H4H28	2	5.1603	4.9648	4.9471	-0.1956	0.0371	-0.1855	-0.0472	0.0000	0.2823
N5C24	2	5.1957	5.1017	5.0981	-0.0939	0.0105	-0.0286	-0.0759	0.0001	0.1262
H3H28	2	5.1958	4.9235	4.8943	-0.2723	0.0369	-0.1620	-0.1473	0.0001	0.3668
N6N20	1	5.2073	5.2295	5.2143	0.0222	0.0090	-0.1983	0.2114	0.0001	0.1522
N6C21	2	5.2791	5.2329	5.2255	-0.0463	0.0114	-0.1407	0.0831	-0.0001	0.1429
C1H27	2	5.2997	5.2583	5.2502	-0.0413	0.0331	-0.0050	-0.0695	0.0001	0.2132
N5H28	2	5.3275	4.9999	4.9766	-0.3276	0.0285	-0.0181	-0.3380	0.0000	0.2816
C1H30	2	5.3857	5.5112	5.5051	0.1255	0.0284	-0.1114	0.2086	-0.0001	0.1642
N5H27	2	5.3918	5.1887	5.1663	-0.2031	0.0391	0.0493	-0.2915	0.0000	0.3094
C7H22	2	5.4585	5.3374	5.3243	-0.1211	0.0225	-0.1872	0.0437	-0.0001	0.2247
H4H30	2	5.4934	5.7149	5.6971	0.2215	0.0313	-0.1660	0.3562	0.0000	0.2526
H4H27	2	5.5595	5.6016	5.5899	0.0421	0.0304	-0.0054	0.0171	0.0000	0.2504
N6H22	2	5.5698	5.5111	5.4865	-0.0587	0.0141	-0.2811	0.2083	0.0000	0.2137
H4H26	2	5.6656	5.7768	5.7643	0.1112	0.0272	-0.0933	0.1773	0.0000	0.2653
C7C21	1	5.6885	5.5633	5.5594	-0.1252	0.0038	-0.0585	-0.0706	0.0001	0.1461
C1H26	2	5.7243	5.7381	5.7348	0.0138	0.0239	-0.0893	0.0791	0.0001	0.1353
H3C23	2	5.7996	5.8187	5.8164	0.0191	0.0158	-0.0516	0.0549	0.0000	0.1158
H8H25	2	5.7999	5.4691	5.4161	-0.3308	0.0431	-0.3251	-0.0489	0.0001	0.4375
H3H25	2	5.8266	5.8305	5.8239	0.0039	0.0309	-0.0523	0.0253	0.0000	0.1967
H11H25	1	5.8327	5.3637	5.3075	-0.4690	0.0755	-0.0245	-0.5201	0.0001	0.5317
H8H22	1	5.8417	5.6951	5.6497	-0.1466	0.0169	-0.4001	0.2366	0.0000	0.2814
N6H29	2	5.8418	6.1996	6.1873	0.3578	0.0284	0.0038	0.3256	0.0000	0.2769
N6H28	2	5.8451	5.6016	5.5846	-0.2435	0.0432	-0.0868	-0.1999	0.0000	0.3035
N6H25	2	5.9184	5.6799	5.6516	-0.2385	0.0284	-0.2246	-0.0423	0.0000	0.3414
H3H30	2	5.9481	6.1619	6.1527	0.2138	0.0278	-0.1115	0.2975	0.0000	0.2189
N6C24	2	5.9494	5.9737	5.9711	0.0243	0.0212	-0.0796	0.0827	0.0000	0.1257
H8H28	2	5.9771	5.7067	5.6848	-0.2704	0.0510	-0.0334	-0.2880	0.0000	0.3047
H8H27	2	6.0047	5.7254	5.6948	-0.2793	0.0552	-0.1162	-0.2183	0.0000	0.4260
H8C23	2	6.0677	5.7955	5.7722	-0.2722	0.0319	-0.2241	-0.0801	0.0001	0.3204
N5H26	2	6.0724	5.8838	5.8774	-0.1886	0.0282	-0.1118	-0.1050	0.0000	0.1982
N6C23	2	6.1156	5.9354	5.9236	-0.1802	0.0176	-0.1636	-0.0342	0.0000	0.2212
C7H25	2	6.1328	5.8338	5.8133	-0.2990	0.0257	-0.0390	-0.2857	0.0000	0.3317

H3H27	2	6.1566	6.1228	6.1149	-0.0339	0.0308	-0.0471	-0.0175	-0.0001	0.2287
N6H27	2	6.1787	5.9782	5.9584	-0.2005	0.0357	-0.0962	-0.1401	0.0001	0.3449
N5H30	2	6.1797	6.1018	6.0990	-0.0779	0.0222	-0.0935	-0.0066	0.0000	0.1427
H8C24	2	6.1959	6.1394	6.1340	-0.0565	0.0265	-0.0762	-0.0068	0.0000	0.1857
H8H29	2	6.2523	6.5345	6.5196	0.2822	0.0277	0.0091	0.2454	0.0000	0.2992
C7H29	2	6.4429	6.6607	6.6528	0.2178	0.0179	-0.0299	0.2298	0.0000	0.2320
C9H25	2	6.4706	6.0109	5.9720	-0.4597	0.0398	0.0167	-0.5162	0.0000	0.4315
C7C23	2	6.5062	6.2517	6.2420	-0.2545	0.0089	-0.0309	-0.2325	0.0000	0.2262
H15H29	1	6.5335	7.1199	7.1045	0.5864	0.0546	-0.0334	0.5652	0.0000	0.3506
C7C24	2	6.5798	6.5160	6.5134	-0.0638	0.0072	-0.0573	-0.0137	0.0000	0.1226
H3H26	2	6.6128	6.6743	6.6703	0.0615	0.0207	-0.0985	0.1393	0.0000	0.1605
H11H27	2	6.6320	6.1851	6.1136	-0.4469	0.0439	0.1748	-0.6656	0.0000	0.4893
C7H28	2	6.6806	6.3575	6.3406	-0.3231	0.0192	-0.0628	-0.2794	-0.0001	0.2917
C7H27	2	6.7685	6.4878	6.4635	-0.2807	0.0175	0.0386	-0.3368	0.0000	0.3431
C10H29	2	7.0045	7.3041	7.2958	0.2995	0.0338	-0.0867	0.3524	0.0000	0.2528
N6H30	2	7.0048	7.0014	6.9983	-0.0033	0.0295	-0.1479	0.1151	0.0000	0.1371
C9C23	1	7.0479	6.6313	6.6067	-0.4166	0.0156	0.0228	-0.4550	0.0000	0.3297
H8H26	2	7.1329	6.8458	6.8252	-0.2872	0.0321	-0.2795	-0.0398	0.0000	0.3134
N6H26	2	7.1375	6.9646	6.9542	-0.1729	0.0221	-0.2153	0.0202	0.0001	0.2104
H14H29	2	7.1989	7.1411	7.1192	-0.0578	0.0414	-0.1878	0.0887	-0.0001	0.3949
H8H30	2	7.2286	7.0835	7.0784	-0.1450	0.0330	-0.1624	-0.0156	0.0000	0.2027
C10H25	2	7.2781	7.0256	7.0080	-0.2524	0.0096	0.0120	-0.2741	0.0001	0.2735
C9H27	2	7.2925	6.8607	6.8111	-0.4318	0.0184	0.1331	-0.5833	0.0000	0.4168
H11H28	2	7.2942	6.8960	6.8553	-0.3982	0.0191	0.0976	-0.5150	0.0001	0.3121
C10C24	1	7.3456	7.3671	7.3645	0.0215	0.0168	-0.1100	0.1147	0.0000	0.1445
H11H29	2	7.4441	7.4566	7.4406	0.0125	0.0118	0.0026	-0.0018	-0.0001	0.3066
H11H26	2	7.4676	6.9713	6.9372	-0.4963	0.0366	-0.0914	-0.4415	0.0000	0.4660
C7H26	2	7.4736	7.2220	7.2140	-0.2517	0.0151	-0.1087	-0.1581	0.0000	0.2323
C10H28	2	7.5496	7.2572	7.2424	-0.2925	0.0233	-0.1655	-0.1502	-0.0001	0.3259
C7H30	2	7.5782	7.5317	7.5292	-0.0465	0.0176	-0.1140	0.0499	0.0000	0.1445
C9C24	2	7.5862	7.3882	7.3809	-0.1981	0.0025	-0.0203	-0.1802	-0.0001	0.1730
C9H29	2	7.6019	7.6756	7.6677	0.0737	0.0093	-0.0213	0.0857	0.0000	0.2324
C9H28	2	7.6715	7.2742	7.2506	-0.3973	0.0106	0.0178	-0.4257	0.0000	0.2747
H13H27	1	7.6732	7.1852	7.1054	-0.4880	0.0150	0.2295	-0.7325	0.0000	0.4725
H14H28	1	7.8944	7.3541	7.3298	-0.5403	0.0259	-0.2216	-0.3446	0.0000	0.4180
H13H29	2	7.9448	7.9069	7.8933	-0.0379	0.0159	-0.0331	-0.0207	0.0000	0.3193
C10H27	2	7.9471	7.7132	7.6963	-0.2339	0.0072	0.0044	-0.2455	0.0000	0.3018
H15H30	2	8.0041	8.4132	8.4038	0.4091	0.0415	-0.1069	0.4745	0.0000	0.2767
C9H26	2	8.0225	7.5755	7.5550	-0.4470	0.0187	-0.0746	-0.3911	0.0000	0.3561
H13H28	2	8.1647	7.7063	7.6744	-0.4584	0.0119	0.0335	-0.5037	-0.0001	0.3479
H11H30	2	8.1905	7.8602	7.8441	-0.3303	0.0164	-0.0679	-0.2788	0.0000	0.3105
H12H27	2	8.1924	7.7449	7.7042	-0.4475	0.0222	0.0288	-0.4984	-0.0001	0.4553
C10H30	2	8.3330	8.4401	8.4366	0.1072	0.0263	-0.1437	0.2245	0.0001	0.1748
H12H29	2	8.4657	8.6196	8.6118	0.1539	0.0178	-0.0644	0.2005	0.0000	0.2515
H14H30	2	8.4673	8.3298	8.3153	-0.1375	0.0323	-0.1862	0.0164	0.0000	0.3477
C10H26	2	8.4799	8.3164	8.3106	-0.1635	0.0112	-0.0870	-0.0878	0.0001	0.1883
H12H28	2	8.4895	8.1217	8.1020	-0.3678	0.0192	-0.0578	-0.3292	0.0000	0.3062
C9H30	2	8.5326	8.3028	8.2962	-0.2298	0.0112	-0.0858	-0.1551	-0.0001	0.2057
H13H30	2	8.8329	8.5614	8.5450	-0.2715	0.0149	-0.0459	-0.2405	0.0000	0.3349
H12H26	1	9.0223	8.5572	8.5390	-0.4651	0.0210	-0.1624	-0.3237	0.0000	0.3763
H16H30	1	9.3409	9.4869	9.4829	0.1460	0.0343	-0.1851	0.2968	0.0000	0.1903
H12H30	2	9.4592	9.2548	9.2491	-0.2044	0.0183	-0.1543	-0.0685	0.0001	0.2188

Table S6. Cartesian coordinates of the *meso* form of tetramezine obtained at the GED(MP2) refinement.

Atom	X	Y	Z
C1	-0.007311	0.021446	-0.004011
C2	0.005827	-0.023149	1.525330
H3	0.841051	-0.534928	-0.385588
H4	0.063114	1.053506	-0.335639
N5	-1.278248	-0.501684	-0.430356
N6	-1.161774	-1.990293	-0.682332
C7	-1.372242	-1.044096	-1.745693
H8	-2.070325	-2.350833	-0.400342
C9	-2.745106	-0.927578	-2.383096
C10	-0.271046	-0.908598	-2.782622
H11	-3.499402	-0.943652	-1.606209
H12	-2.903801	-1.749091	-3.074156
H13	-2.819003	0.006886	-2.928825
H14	-0.255930	0.104838	-3.170578
H15	0.693175	-1.158497	-2.368035
H16	-0.482567	-1.587271	-3.601385
H17	-0.842534	0.533225	1.906907
H18	-0.064598	-1.055209	1.856958
N19	1.276765	0.499981	1.951676
N20	1.160291	1.988590	2.203652
C21	1.370758	1.042393	3.267012
H22	2.068842	2.349130	1.921662
C23	2.743622	0.925875	3.904415
C24	0.269562	0.906895	4.303941
H25	3.497918	0.941949	3.127529
H26	2.902317	1.747388	4.595475
H27	2.817519	-0.008589	4.450144
H28	0.254446	-0.106541	4.691897
H29	-0.694658	1.156794	3.889354
H30	0.481084	1.585568	5.122704

Table S7. Cartesian coordinates of the *enantiomeric* form of tetramezine obtained at the GED(MP2) refinement.

Atom	X	Y	Z
C1	0.019912	0.025409	-0.002608
C2	0.021762	-0.024236	1.526606
H3	0.955036	-0.386146	-0.369378
H4	-0.066800	1.058326	-0.327816
N5	-1.129629	-0.696557	-0.479184
N6	-0.754023	-2.144518	-0.713958
C7	-1.074654	-1.247703	-1.792973
H8	-1.600815	-2.650644	-0.465499
C9	-2.420643	-1.362293	-2.485970
C10	0.029122	-0.936359	-2.789280
H11	-3.192227	-1.497765	-1.738313
H12	-2.414095	-2.201966	-3.173529
H13	-2.624816	-0.455180	-3.044658
H14	-0.105579	0.065414	-3.184501
H15	1.005886	-1.026527	-2.339889
H16	-0.038534	-1.641603	-3.610177
H17	0.956863	0.389321	1.891177
H18	-0.061973	-1.057335	1.852014
N19	-1.128197	0.695269	2.005885
N20	-0.755141	2.144032	2.239779
C21	-1.071314	1.246534	3.319542
H22	-1.603597	2.648343	1.993312
C23	-2.415913	1.358245	4.015701
C24	0.035464	0.937557	4.313250
H25	-3.189541	1.492063	3.269861
H26	-2.409546	2.197931	4.703245
H27	-2.616830	0.450698	4.574866
H28	-0.096162	-0.064501	4.708785
H29	1.010974	1.029815	3.861565
H30	-0.031770	1.642656	5.134306

Table S8. Cartesian coordinates of the *meso* form of tetramezine obtained at the GED(B3LYP) refinement.

Atom	X	Y	Z
C1	0.017524	0.019693	-0.004014
C2	-0.017524	-0.019693	1.525335
H3	0.885018	-0.522801	-0.367365
H4	0.084444	1.049751	-0.345950
N5	-1.243649	-0.520681	-0.448709
N6	-1.158630	-2.001417	-0.721708
C7	-1.370811	-1.040437	-1.769940
H8	-2.056540	-2.375325	-0.420837
C9	-2.776648	-0.903158	-2.328454
C10	-0.238297	-0.927031	-2.775635
H11	-3.478255	-0.923000	-1.502805
H12	-2.963178	-1.722353	-3.017700
H13	-2.853947	0.042698	-2.856991
H14	-0.226631	0.081932	-3.178565
H15	0.704507	-1.164521	-2.305130
H16	-0.435457	-1.634021	-3.575667
H17	-0.885018	0.522801	1.888686
H18	-0.084444	-1.049751	1.867271
N19	1.243649	0.520681	1.970030
N20	1.158630	2.001417	2.243029
C21	1.370811	1.040437	3.291261
H22	2.056540	2.375325	1.942158
C23	2.776648	0.903158	3.849775
C24	0.238297	0.927031	4.296956
H25	3.478255	0.923000	3.024126
H26	2.963178	1.722353	4.539021
H27	2.853947	-0.042698	4.378312
H28	0.226631	-0.081932	4.699886
H29	-0.704507	1.164521	3.826451
H30	0.435457	1.634021	5.096988

Table S9. Cartesian coordinates of the *enantiomeric* form of tetramezine obtained at the GED(B3LYP) refinement.

Atom	X	Y	Z
C1	0.045524	0.026558	-0.002736
C2	0.045524	-0.026558	1.526782
H3	0.999300	-0.344826	-0.369715
H4	-0.073376	1.054380	-0.336329
N5	-1.079873	-0.741160	-0.476723
N6	-0.692236	-2.167229	-0.775124
C7	-1.081816	-1.246650	-1.809157
H8	-1.499552	-2.721201	-0.496130
C9	-2.479261	-1.385454	-2.388478
C10	0.015577	-0.888241	-2.797207
H11	-3.172057	-1.562050	-1.574205
H12	-2.487371	-2.211884	-3.094226
H13	-2.739443	-0.464521	-2.902484
H14	-0.175702	0.107734	-3.187157
H15	0.983082	-0.934916	-2.318907
H16	-0.023551	-1.608083	-3.609081
H17	0.999300	0.344826	1.893761
H18	-0.073376	-1.054380	1.860375
N19	-1.079873	0.741160	2.000769
N20	-0.692236	2.167229	2.299170
C21	-1.081816	1.246650	3.333203
H22	-1.499552	2.721201	2.020176
C23	-2.479261	1.385454	3.912524
C24	0.015577	0.888241	4.321253
H25	-3.172057	1.562050	3.098251
H26	-2.487371	2.211884	4.618272
H27	-2.739443	0.464521	4.426530
H28	-0.175702	-0.107734	4.711203
H29	0.983082	0.934916	3.842953
H30	-0.023551	1.608083	5.133127

Table S10. Correlation matrix for the GED (B3LYP) refinement of the geometrical parameters united in the independent groups.

	CC	**NN**	**C_{Me}–C–C_{Me}**	**CN**	**C_{Eth}–C_{Eth}–N**	**H–C_{Me}–H**	**CH**
CC	1.0000						
NN	-0.6595	1.0000					
C_{Me}–C–C_{Me}	0.2481	-0.4553	1.0000				
CN	-0.6139	0.1118	0.3206	1.0000			
C_{Eth}–C_{Eth}–N	0.2484	-0.2937	-0.1959	-0.3047	1.0000		
H–C_{Me}–H	-0.1333	0.1274	0.2979	0.1760	-0.8974	1.0000	
CH	0.3757	-0.1276	-0.0758	-0.4839	0.1524	0.1113	1.0000

Table S11. Correlation matrix for the GED (MP2) refinement of the geometrical parameters united in the independent groups.

	CC	NN	C_{Me}–C–C_{Me}	CN	C_{Eth}–C_{Eth}–N	H–C_{Me}–H	CH
CC	1.0000						
NN	-0.6995	1.0000					
C_{Me}–C–C_{Me}	0.1749	-0.3443	1.0000				
CN	-0.5813	0.1107	0.3879	1.0000			
C_{Eth}–C_{Eth}–N	0.3319	-0.3455	-0.4443	-0.3290	1.0000		
H–C_{Me}–H	-0.2411	0.2265	0.5090	0.2551	-0.8955	1.0000	
CH	0.3653	-0.1154	-0.0629	-0.4808	0.0395	0.1189	1.0000

5. Results of quantum-chemical calculations

Table S12. Cartesian coordinates of the *meso* form of tetramezine found by the MP2/cc-pVTZ calculation.

Atom	X	Y	Z
C1	-0.019015261	0.0199803361	0.006543227
C2	0.019015261	-0.0199803361	1.514777773
H3	0.8303590663	-0.5336887387	-0.3821103807
H4	0.0463793023	1.0549619285	-0.3232990225
N5	-1.297336587	-0.5075175112	-0.434547364
N6	-1.1775226829	-1.9819857461	-0.6864394161
C7	-1.3840632361	-1.0375062861	-1.7689454036
H8	-2.0873115901	-2.3441864909	-0.4106370059
C9	-2.7528736743	-0.9292981465	-2.366046757
C10	-0.2598036003	-0.9072058311	-2.7500273264
H11	-3.498614722	-0.9492254416	-1.5783856349
H12	-2.9338975519	-1.7482895303	-3.0576304514
H13	-2.8554463375	0.004247993	-2.9125304155
H14	-0.2164061168	0.1057266142	-3.1425173524
H15	0.693934857	-1.160993492	-2.3093734601
H16	-0.4344072219	-1.5808241301	-3.5840730876
H17	-0.8303590663	0.5336887387	1.9034313807
H18	-0.0463793023	-1.0549619285	1.8446200225
N19	1.297336587	0.5075175112	1.955868364
N20	1.1775226829	1.9819857461	2.2077604161
C21	1.3840632361	1.0375062861	3.2902664036
H22	2.0873115901	2.3441864909	1.9319580059
C23	2.7528736743	0.9292981465	3.887367757
C24	0.2598036003	0.9072058311	4.2713483264
H25	3.498614722	0.9492254416	3.0997066349
H26	2.9338975519	1.7482895303	4.5789514514
H27	2.8554463375	-0.004247993	4.4338514155
H28	0.2164061168	-0.1057266142	4.6638383524
H29	-0.693934857	1.160993492	3.8306944601
H30	0.4344072219	1.5808241301	5.1053940876

Table S13. Cartesian coordinates of the *enantiomeric* form of tetramezine found by the MP2/cc-pVTZ calculation.

Atom	X	Y	Z
C1	-0.0014800069	0.018632132	0.007644832
C2	-0.0014800069	-0.018632132	1.516401168
H3	0.9387857439	-0.3950637696	-0.3491238088
H4	-0.0835396154	1.0531983257	-0.319940603
N5	-1.1517313381	-0.7047505671	-0.5018992994
N6	-0.7779250514	-2.1405008036	-0.7266890299
C7	-1.070550266	-1.2459626483	-1.8320099144
H8	-1.6317884021	-2.6439893192	-0.4978441588
C9	-2.4019744739	-1.3633802571	-2.5071735515
C10	0.0720739252	-0.9433588652	-2.7528498604
H11	-3.1784834745	-1.4957484876	-1.7612774635
H12	-2.4098744194	-2.2059111043	-3.194255346
H13	-2.62037499	-0.4622602428	-3.0738554642
H14	-0.0229097778	0.0620523623	-3.155580665
H15	1.0294655845	-1.0423535787	-2.2610165522
H16	0.0516425619	-1.6394471669	-3.586534717
H17	0.9387857439	0.3950637696	1.8731698088
H18	-0.0835396154	-1.0531983257	1.843986603
N19	-1.1517313381	0.7047505671	2.0259452994
N20	-0.7779250514	2.1405008036	2.2507350299
C21	-1.070550266	1.2459626483	3.3560559144
H22	-1.6317884021	2.6439893192	2.0218901588
C23	-2.4019744739	1.3633802571	4.0312195515
C24	0.0720739252	0.9433588652	4.2768958604
H25	-3.1784834745	1.4957484876	3.2853234635
H26	-2.4098744194	2.2059111043	4.718301346
H27	-2.62037499	0.4622602428	4.5979014642
H28	-0.0229097778	-0.0620523623	4.679626665
H29	1.0294655845	1.0423535787	3.7850625522
H30	0.0516425619	1.6394471669	5.110580717

Table S14. Cartesian coordinates of the *meso* form of tetramezine found by the B3LYP/cc-pVTZ calculation.

Atom	X	Y	Z
C1	-0.0134944331	0.0068151326	-0.001125686
C2	0.0134944331	-0.0068151326	1.522446686
H3	0.8571512314	-0.5320880762	-0.378414785
H4	0.0384056908	1.0410094671	-0.3505556296
N5	-1.2827456566	-0.547735023	-0.4654211787
N6	-1.1847284125	-2.0165302399	-0.7359637849
C7	-1.3970918533	-1.0578349402	-1.8114694736
H8	-2.0825504082	-2.3966030191	-0.4426462735
C9	-2.7827179102	-0.9251298167	-2.4032746776
C10	-0.2772390776	-0.9350930493	-2.8206164204
H11	-3.5338970984	-0.9435095486	-1.6148404445
H12	-2.9813266241	-1.7363313245	-3.1070988076
H13	-2.8820691599	0.0178422468	-2.944410884
H14	-0.2503043812	0.0705403856	-3.2453481474
H15	0.6908707717	-1.1610953124	-2.3844981482
H16	-0.4466816607	-1.6359059214	-3.6396554915
H17	-0.8571512314	0.5320880762	1.899735785
H18	-0.0384056908	-1.0410094671	1.8718766296
N19	1.2827456566	0.547735023	1.9867421787
N20	1.1847284125	2.0165302399	2.2572847849
C21	1.3970918533	1.0578349402	3.3327904736
H22	2.0825504082	2.3966030191	1.9639672735
C23	2.7827179102	0.9251298167	3.9245956776
C24	0.2772390776	0.9350930493	4.3419374204
H25	3.5338970984	0.9435095486	3.1361614445
H26	2.9813266241	1.7363313245	4.6284198076
H27	2.8820691599	-0.0178422468	4.465731884
H28	0.2503043812	-0.0705403856	4.7666691474
H29	-0.6908707717	1.1610953124	3.9058191482
H30	0.4466816607	1.6359059214	5.1609764915

Table S15. Cartesian coordinates of the *enantiomeric* form of tetramezine found by the B3LYP /cc-pVTZ calculation.

Atom	X	Y	Z
C1	-0.0017543912	0.0015660669	-0.0000022996
C2	-0.0017543912	-0.0015660669	1.5240482996
H3	0.9643586277	-0.3775223992	-0.3422615386
H4	-0.1139851828	1.0288694544	-0.3547189628
N5	-1.1203113107	-0.7755291491	-0.5285022878
N6	-0.7247997979	-2.1933238686	-0.7972811477
C7	-1.0661334406	-1.2803486868	-1.8798966724
H8	-1.5451880287	-2.7436076021	-0.5510458009
C9	-2.420273544	-1.4119774104	-2.5412230979
C10	0.0559612293	-0.9336275108	-2.8339905309
H11	-3.1910987224	-1.5830413429	-1.7911208565
H12	-2.4227656425	-2.2387722682	-3.2549920323
H13	-2.6733574641	-0.5002290862	-3.0858335383
H14	-0.0950389428	0.0604710714	-3.2600278051
H15	1.0288774266	-0.9681792084	-2.3532474611
H16	0.0668422593	-1.6485032843	-3.6583666047
H17	0.9643586277	0.3775223992	1.8663075386
H18	-0.1139851828	-1.0288694544	1.8787649628
N19	-1.1203113107	0.7755291491	2.0525482878
N20	-0.7247997979	2.1933238686	2.3213271477
C21	-1.0661334406	1.2803486868	3.4039426724
H22	-1.5451880287	2.7436076021	2.0750918009
C23	-2.420273544	1.4119774104	4.0652690979
C24	0.0559612293	0.9336275108	4.3580365309
H25	-3.1910987224	1.5830413429	3.3151668565
H26	-2.4227656425	2.2387722682	4.7790380323
H27	-2.6733574641	0.5002290862	4.6098795383
H28	-0.0950389428	-0.0604710714	4.7840738051
H29	1.0288774266	0.9681792084	3.8772934611
H30	0.0668422593	1.6485032843	5.1824126047