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> Disulphide Bond Exchange Inhibited by Air - Kinetic and Thermodynamic Products in a Library of Macrocyclic Cysteine Derivatives

Agnieszka Cholewiak,<sup>1</sup> Łukasz Dobrzycki,<sup>2</sup> Janusz Jurczak,<sup>1</sup> Filip Ulatowski<sup>1\*</sup>

<sup>1</sup>Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/50 01-224 Warsaw, Poland; <sup>2</sup>Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland; \*filip.ulatowski@icho.edu.pl

## **Supporting Information**

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2. NMR Spectra























Fig. S11 Chromatograms of mixtures obtained upon oxidation of dithios a) 3a, b) 3b, c) 3c, and d) 3d.



Fig. S12 Chromatograms of (a) [7a<sub>1</sub>], after heating for (b) 2h, (c) 4h at 80°C.



S14



Fig. S14 Chromatograms of (a) [7b<sub>1</sub>], after addition of TBAOH: (b) 5 min, (c) 15 min, (d) 60min.



**Fig. S15** Chromatogram of mixture of [**7a**<sub>2</sub>] and [**7b**<sub>2</sub>] 120 min after addition of 20 mol% of thiols **3a** and **3b** and TBAOH.

## 4. X-ray measurments

The X-ray measurement of **[2**<sub>2</sub>] was performed at 100(2) K on a Bruker D8 Venture Photon100 diffractometer equipped with a TRIUMPH monochromator and a MoK $\alpha$  fine focus sealed tube ( $\lambda$  = 0.71073 Å). A total of 1450 frames were collected with Bruker APEX2 program [1]. The frames were integrated with the Bruker SAINT software package [2] using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 22761 reflections to a maximum  $\theta$  angle of 25.49° (0.83 Å resolution), of which 3094 were independent (average redundancy 7.356, completeness = 100.0%, R<sub>int</sub> = 2.26%, R<sub>sig</sub> = 1.39%) and 2777 (89.75%) were greater than 2 $\sigma$ (F<sup>2</sup>). The final cell constants of <u>a</u> = 15.4619(9) Å, <u>b</u> = 9.5378(5) Å, <u>c</u> = 22.6171(12) Å,  $\beta$  = 92.5215(13)°, volume = 3332.2(3) Å<sup>3</sup>, are based upon the refinement of the XYZ-centroids of 9931 reflections above 20  $\sigma$ (I) with 5.019° < 2 $\theta$  < 52.21°. Data were corrected for absorption effects using the multi-scan method (SADABS) [7]. The ratio of minimum to maximum apparent transmission was 0.933. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8320 and 0.9250.

The structure was solved and refined using SHELXTL Software Package [4] using the space group C 1 2/c 1, with Z = 4 for the formula unit,  $C_{26}H_{38}N_6O_6S_6$ . The final anisotropic full-matrix least-squares refinement on F<sup>2</sup> with 209 variables converged at R1 = 2.75%, for the observed data and wR2 = 7.02% for all data. The goodness-of-fit was 1.099. The largest peak in the final difference electron density synthesis was 0.391 e<sup>-</sup>/Å<sup>3</sup> and the largest hole was -0.159 e<sup>-</sup>/Å<sup>3</sup> with an RMS deviation of 0.055 e<sup>-</sup>/Å<sup>3</sup>. On the basis of the final model, the calculated density was 1.441 g/cm<sup>3</sup> and F(000), 1520 e<sup>-</sup>.

The non-hydrogen atoms were refined anisotropically. Most of hydrogen atoms were placed in calculated positions and refined within the riding model. The temperature factors of these hydrogen atoms were not refined and were set to be equal to either 1.2 or 1.5 times larger than  $U_{eq}$  of the corresponding heavy atom. Positions of two hydrogen atoms engaged in hydrogen bonds were refined together with their isotropic temperature factors. The atomic scattering factors were taken from the International Tables [5].

These data are deposited at CCDC base under number CCDC 1551580

The X-ray measurement of **[7a<sub>2</sub>]** was performed at 100(2) K on a Bruker D8 Venture Photon100 diffractometer equipped with a TRIUMPH monochromator and a MoK $\alpha$  fine focus sealed tube ( $\lambda$  = 0.71073 Å). A total of 870 frames were collected with Bruker APEX2 program [1]. The frames were integrated with the Bruker SAINT software package [2] using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 210438 reflections to a maximum  $\vartheta$  angle of 25.05° (0.84 Å resolution), of which 30740 were independent, but not fully merged due to twinning and HKLF5 format of the data (average redundancy 6.84, completeness = 99.9%, R<sub>int</sub> = 10.44%, R<sub>sig</sub> = 11.59%). 20093 reflections (65.36%) were greater than  $2\sigma(F^2)$ . The final cell constants of a = 19.763(2) Å, b = 21.594(2) Å, c = 33.712(4) Å, V = 14387.(3) Å<sup>3</sup>, are based upon the refinement of the XYZ-centroids of 9331 reflections above 20  $\sigma(I)$  with 4.465° < 2 $\vartheta$  < 40.06°. Data were

corrected for absorption effects using the multi-scan method (TWINABS) [6]. The ratio of minimum to maximum apparent transmission was 0.759. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.893 and 0.968.

The structure was solved and refined using SHELXTL Software Package [4] using the space group  $P2_12_12_1$ , with Z = 4 for the formula unit,  $C_{124.40}H_{156.62}N_{20}O_{25.40}S_{16.20}$ . and the Flack parameter equal to 0.00(4) [7]. The final anisotropic full-matrix least-squares refinement on  $F^2$  with 2035 variables converged at R1 = 9.64%, for the observed data and wR2 = 25.99% for all data. The goodness-of-fit was 1.091. The largest peak in the final difference electron density synthesis was 0.560 e<sup>-</sup>/Å<sup>3</sup> and the largest hole was -0.427 e<sup>-</sup>/Å<sup>3</sup> with an RMS deviation of 0.080 e<sup>-</sup>/Å<sup>3</sup>. On the basis of the final model, the calculated density was 1.319 g/cm<sup>3</sup> and F(000), 6022 e<sup>-</sup>.

The investigated crystal is twinned by reticular pseudomerohedry, with partial overlap of some reflection. Due to twinning effect data integration and scaling was based on two domains resulting the HKLF5 format of the reflection data. The refined twin fractions are equal to 0.732(2) and 0.268(2). In addition the structure is heavily disordered thus resulting in weak scattering power, especially at higher  $2\vartheta$  diffraction angles. In spite of the disorder, twinning effects and use of MoK $\alpha$  X-ray radiation the diffraction experiment confirmed optical purity of investigated compound. It was possible due to relatively high sulfur atoms contents coming from both the macrocycle compound and large amount of dimethyl sulfoxide (DMSO) solvent molecules in the crystal lattice. The compound crystallizes the chiral  $P2_12_12_1$  space group with Flack parameter equal to 0.00(4) with both twin components belonging to the same enantiomorphic phase.

The structure in the asymmetric part of the unit cell contains two macrocycle molecules, 8.2 DMSO molecules and 1.2 species of  $H_2O$ . In the latter case H atoms were not assigned. As mentioned above structure is severely disordered with many atoms both in macrocycle molecules and the solvent moieties disordered over two sites. In most cases the occupancy ratios of both disordered fragments were refined. DMSO molecules is located in 9 sites, with only one moiety fully ordered. Among the other DMSO molecules 6 sites are fully occupied whereas in two cases the sum occupation of the atoms is equal to 0.5 and 0.7. The occupancy of the water molecules located at three sites, in the asymmetric part of the unit cell, is equal to 0.6, 0.3 and 0.3. To preserve reasonable geometry of disordered fragments number of restraints was applied.

All ordered non-hydrogen atoms and major component (occupancy  $\geq$ 50%) disordered non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in calculated positions and refined within the riding model. The temperature factors of the hydrogen atoms were not refined and were set to be equal to either 1.2 or 1.5 times larger than U<sub>eq</sub> of the corresponding heavy atom. The atomic scattering factors were taken from the International Tables [5].

These data are deposited at CCDC base under number CCDC 1551754

## 5. Coordinates of optimised geometries

Compo	ound <b>1</b> , conforma	tion A:	
Н	-4.049355	2.611814	-0.206692
С	-3.209553	1.925624	-0.153145
N	-1.050411	0.163603	-0.017308
С	-2.685212	1.542878	1.079981
С	-2.641493	1.410800	-1.316648
С	-1.563341	0.528655	-1.198916
С	-1.601583	0.660018	1.097989
Н	-3.090084	1.909145	2.015774
Н	-3.011179	1.670478	-2.301651

ССИНИСИНСИНСИН КИЗИ	$\begin{array}{c} -1.010891\\ -0.947787\\ 0.054761\\ 0.384300\\ 0.040273\\ 0.304390\\ -1.500007\\ -1.359174\\ 0.851186\\ 1.052193\\ 0.255035\\ 2.195822\\ 2.765331\\ 2.784518\\ 0.796108\\ 0.852454\\ 0.243030\\ 2.226244\\ 2.760022\\ 2.767144\\ 2.065838\\ 1.325099\\ 2.340900\\ 1.655423\end{array}$	0.243638 - $0.052430$ - $0.581820$ - $0.800445$ - $0.946993$ - $1.115404$ 0.641875 0.278225 - $0.985862$ - $2.061904$ - $0.808776$ - $0.254704$ - $0.655367$ - $0.412374$ - $1.583044$ - $2.660089$ - $1.441599$ - $1.631594$ - $1.152736$ 1.577918 1.594466 0.743878 0.692146	2.424452 -2.453430 2.330874 1.397260 -2.234738 -1.270819 3.487663 -3.571601 3.472420 3.404625 4.370452 3.568973 4.412569 2.659495 -3.295870 -3.095129 -4.227204 -3.433929 -4.191221 -2.487607 3.731057 4.857972 -3.847584 -5.008063
Composi	nd <b>1</b> . conform	ation B.	
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С	-2.023709	1.952777	2.597175
N	-0.544678	0.504935	0.729613
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H H	-3.311044 -0 517123	2.414610 1 273082	0.908082 4 007719
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С	1.073962	-0.215701	2.405847
N H	-1.145086	0.518213	-1.903963
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Compour	nd <b>1</b> , conform	ation C:	
Н	-4.021805	2.798287	0.838230
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U	2 101205	_0 021595	0 774735
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С	-3.445322	1.375609	0.653657
C	2 317327	1 588269	2 081756
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Н	3.08559/	2.310866	2.358228
Н	1.924040	1.121847	2.987679
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Н	-2.309117	3.010838	-1.437362
н	1 595473	3 161892	0 402503
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Compoun	d <b>3d,</b> confo	rmation E:	
Н	-2.181322	-4.988653	-1.053754
C	-1 817075	-4 027101	-0 704005
	T.0T/9/0	H.UZ/191	0.104095
IN	-0.895553	-1.550815	0.191693
С	-0.451268	-3.782124	-0.594188
С	-2.712179	-3 017165	-0 362365
_		J. U. I. I. U. J	~ • J U Z J U J

C -0.038939 -2.529069 -0.1 H 0.291035 -4.527704 -0.8	178001
Н 0.291035 -4.527704 -0.8	127122
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N -2.833778 0.532815 0.8	310196
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	532100
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C -0.863882 0.796610 -2.8	306783
	7/3150
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н -0.468571 1.776865 -3.0	J82481
H -0.468571 1.776865 -3.0 H -1.619953 0.468738 -3.5	518876
H     -0.468571     1.776865     -3.0       H     -1.619953     0.468738     -3.5       H     -1.992123     3.807263     -0.6	518876 528696
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7	518876 528696 711700
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7	5182481 518876 528696 711700
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7	518876 528696 711700
H -0.468571 1.776865 -3.0 H -1.619953 0.468738 -3.5 H -1.992123 3.807263 -0.6 H 2.412765 2.239853 1.7 Compound <b>3d</b> , conformation F:	518876 528696 711700
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:   -0.258023   -5.716988   -0.9	082481 518876 528696 711700
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:   -   -     H   0.258023   -5.716988   -0.9     C   0.170844   -4.662300   -0.7	967341 967341 725104
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	082481 518876 528696 711700 067341 725104 L07206
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	082481 518876 528696 711700 067341 725104 L07206 231519
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	967341 725104 0725104 0725104 07206 231519
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	082481 518876 528696 711700 067341 725104 L07206 231519 002718 574978
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	082481 518876 528696 711700 067341 725104 L07206 231519 902718 574978
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	2481 518876 528696 711700 967341 725104 L07206 231519 902718 574978 062469
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	282481 518876 528696 711700 967341 725104 L07206 231519 902718 574978 062469 073938
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	02481 518876 528696 711700 067341 725104 L07206 231519 002718 574978 062469 073938 281550
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	382481     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32481     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	322481     518876     528696     711700     967341     725104     L07206     231519     902718     574978     062469     073938     281550     581756     736364     754432
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound 3d, conformation F:H $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.75$ O $3.383415$ $-2.283078$ $0.75$	382481     518876     518876     528696     711700     367341     725104     L07206     231519     302718     574978     362469     073938     281550     581756     736364     754432     77509
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F:H $0.258023$ $-5.716988$ $-0.5$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.2$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7$ O $-3.420956$ $-2.419542$ $-1.5$	322481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     962469     973938     281550     581756     736364     754432     177509     236919
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F:H $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.256674$ C $1.268674$ $-3.957569$ $-0.256966666666666666666666666666666666666$	382481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364     754432     177509     336819
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F:H $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7$ O $-3.420956$ $-2.419542$ $-1.72$ N $1.949875$ $-0.498272$ $0.8$ H $1.023573$ $-0.191200$ $0.5$	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364     754432     177509     336819     577541
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364     754432     177509     336819     557541     347365
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364     754432     177509     336819     557541     347365     037242
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F:H $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.5$ C $0.170844$ $-4.662300$ $-0.5$ C $1.268674$ $-3.957569$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7236373$ O $-3.420956$ $-2.419542$ $-1.2231474$ N $1.949875$ $-0.498272$ $0.87543$ N $1.949875$ $-0.498272$ $0.87543$ N $1.949875$ $-0.236350$ $-0.675743$ N $-2.334714$ $-0.587543$ $-0.57543$ H $-1.437095$ $-0.236350$ $-0.675743$	322481     518876     518876     528696     711700     967341     725104     L07206     231519     902718     574978     062469     073938     281550     581756     736364     754432     L77509     336819     557541     347365     037242     L76600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	382481     518876     518876     528696     711700     967341     725104     102718     502718     502718     502718     502718     575938     281550     581756     736364     754432     177509     336819     557541     347365     37242     176600     731084
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F:H $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.69266666666666666666666666666666666666$	382481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281756     736364     754432     177509     336819     557541     347365     037242     176600     731084     452829
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F:H $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.25$ C $1.268674$ $-3.957569$ $-0.25$ C $-1.041120$ $-3.995503$ $-0.5503$ C $-1.042059$ $-4.429402$ $-0.560495$ H $-1.924059$ $-4.429402$ $-0.560495$ C $-2.400924$ $-1.880439$ $-0.7503$ O $-3.383415$ $-2.283078$ $0.75030$ O $-3.420956$ $-2.419542$ $-1.550743$ N $1.949875$ $-0.498272$ $0.85033$ N $-2.334714$ $-0.587543$ $-0.550743$ H $-1.437095$ $-0.236350$ $-0.670723$ H $-1.437095$ $-0.236350$ $-0.670763$ H $-1.437095$ $-0.236350$ $-0.670763$ H	322481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364     754432     1756364     336819     557541     347365     037242     176600     731084     452829
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F: $H$ $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.9$ C $-1.041120$ $-3.995503$ $-0.5$ C $1.106472$ $-2.638851$ $-0.66276666666666666666666666666666666666$	322481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     962469     973938     281550     581756     736364     754432     177509     336819     557541     347365     37242     176600     731084     452829     315754
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F: $-0.054001$ $-1.957908$ $-0.5$ C $0.170844$ $-4.662300$ $-0.5$ C $1.268674$ $-3.957569$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.041120$ $-3.995503$ $-0.5$ C $1.106472$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7$ O $3.383415$ $-2.283078$ $0.7$ O $-3.420956$ $-2.419542$ $-1.2587543$ N $1.949875$ $-0.498272$ $0.857543$ H $-1.437095$ $-0.236350$ $-0.676496$ H $3.733090$ $0.013835$ $1.7564366666666666666666666666666666666666$	322481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     962469     973938     281550     581756     736364     754432     177509     336819     557541     347365     037242     176600     731084     452829     315754     946499
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F: $H$ $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.9$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7$ O $-3.420956$ $-2.419542$ $-1.22$ N $1.949875$ $-0.498272$ $0.8$ H $1.023573$ $-0.191200$ $0.5$ N $-2.334714$ $-0.587543$ $-0.23$ H $-1.437095$ $-0.236350$ $-0.6$ H $3.733090$ $0.013835$ $1.7$ C $-3.453703$ $0.318896$ $-0.4$ H $-4.370013$ $-0.270793$ $-0.336356$ C $-3.445322$ $1.375609$ $0.6$	32481     518876     518876     528696     711700     967341     725104     L07206     231519     902718     574978     062469     073938     281550     581756     736364     754432     L77509     336819     557541     347365     037242     L76600     731084     452829     315754     046499     553657
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F: $H$ $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.9$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7$ O $-3.420956$ $-2.419542$ $-1.52$ N $1.949875$ $-0.498272$ $0.8$ H $1.023573$ $-0.191200$ $0.52$ N $-2.334714$ $-0.587543$ $-0.52$ H $-1.437095$ $-0.236350$ $-0.62$ H $-1.437095$ $-0.236350$ $-0.62$ H $-1.437013$ $-0.270793$ $-0.52$ C $-3.453703$ $0.318896$ $-0.42$ H $-0.3577042$ $1.588269$ $2.62$	322481     518876     518876     528696     711700     967341     725104     L07206     902718     574978     902718     574978     902718     574978     902718     574978     902718     574078     91550     581756     336819     557541     347365     37242     176600     731084     452829     315754     946499     553657     981756
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F: $H$ $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.5$ C $0.170844$ $-4.662300$ $-0.5$ C $0.170844$ $-4.662300$ $-0.5$ C $1.268674$ $-3.957569$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.2$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7$ O $3.383415$ $-2.283078$ $0.7$ O $-3.420956$ $-2.419542$ $-1.5$ N $1.949875$ $-0.498272$ $0.8$ H $1.023573$ $-0.191200$ $0.5$ N $-2.334714$ $-0.587543$ $-0.7$ H $-1.437095$ $-0.236350$ $-0.6$ H $-3.73090$ $0.13835$ $1.7$ C $-3.453703$ $0.318896$ $-0.4$ H $-4.370013$	322481     518876     518876     528696     711700     967341     725104     107206     231519     902718     502469     902718     502469     902718     502469     902718     562469     973938     281550     581756     736364     754432     177509     336819     557541     347365     037242     176600     731084     452829     315754     953657     953657     953657     953657     958228
H   -0.468571   1.776865   -3.0     H   -1.619953   0.468738   -3.5     H   -1.992123   3.807263   -0.6     H   2.412765   2.239853   1.7     Compound   3d, conformation F:	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     02463     231550     57541     347365     037242     175600     731084     452829     315754     046499     553657     081756     358228     987679
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F:H $0.258023$ $-5.716988$ $-0.6$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.25$ C $1.268674$ $-3.957569$ $-0.25$ C $-1.041120$ $-3.995503$ $-0.65$ C $-2.231445$ $-4.429402$ $-0.66$ H $2.221445$ $-4.429402$ $-0.66$ H $-1.924059$ $-4.497311$ $-1.22$ C $-2.334714$ $-0.587543$ $-0.56$ N $-2.334714$ $-0.587543$ $-0.56$ N $-2.334714$ $-0.587543$ $-0.56$ H $-1.437095$ $-0.236350$ $-0.66$ H $-3.73090$ $0.13835$ $1.76$ C $-3.445322$ $1.375609$ $0.66$ H $-3.085597$ $2.310866$ $2.56751$ <td>32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364     754432     1756364     336819     557541     347365     037242     176600     452829     315754     046499     653657     037242     17563     35754     037242     176600     731084     452829     315754     0365764     037242     176600     35828     037242     17563     037242     17563     037242     17563     037242     17563     037242     037528     0387679</td>	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     062469     073938     281550     581756     736364     754432     1756364     336819     557541     347365     037242     176600     452829     315754     046499     653657     037242     17563     35754     037242     176600     731084     452829     315754     0365764     037242     176600     35828     037242     17563     037242     17563     037242     17563     037242     17563     037242     037528     0387679
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F: $H$ $0.258023$ $-5.716988$ $-0.9$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.2$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.9$ C $-1.041120$ $-3.995503$ $-0.9$ C $-1.041120$ $-3.995503$ $-0.9$ C $-1.041120$ $-3.995503$ $-0.9$ C $1.106472$ $-2.638851$ $-0.9$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.334714$ $-0.587543$ $-0.7569$ O $3.383415$ $-2.283078$ $0.7569$ O $-3.420956$ $-2.419542$ $-1.226350$ N $1.949875$ $-0.498272$ $0.857666$ N $-2.334714$ $-0.587543$ $-0.75669$ N $-2.334714$ $-0.587543$ $-0.76666$ H $3.733090$ $0.013835$ $1.76669$ H $-4.370013$ $-0.270793$ $-0.7666666666666666666666666666666666666$	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     962469     973938     281550     581756     736364     754432     177509     336819     557541     347365     37242     176600     731084     452829     315754     946499     553657     987679     987679     987679     987679
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound 3d, conformation F: $H$ $0.258023$ $-5.716988$ $-0.6$ C $0.170844$ $-4.662300$ $-0.7$ N $-0.054001$ $-1.957908$ $-0.7$ C $1.268674$ $-3.957569$ $-0.2$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.041120$ $-3.995503$ $-0.5$ C $-1.104792$ $-2.638851$ $-0.5$ C $1.106472$ $-2.601451$ $0.6$ H $2.231445$ $-4.429402$ $-0.6$ H $-1.924059$ $-4.497311$ $-1.22$ C $2.266357$ $-1.788665$ $0.5$ C $-2.400924$ $-1.880439$ $-0.7$ O $3.383415$ $-2.283078$ $0.7$ O $3.383415$ $-2.283078$ $0.7$ O $3.383415$ $-2.283078$ $0.7$ O $-3.420956$ $-2.419542$ $-1.27$ N $1.949875$ $-0.498272$ $0.8$ H $1.023573$ $-0.191200$ $0.5$ N $-2.334714$ $-0.587543$ $-0.7$ C $2.3453703$ $0.318896$ $-0.4$ H $-3.63703$ $0.318896$ $-0.4$ H $-3.630033$ $0.207269$ $2.5$	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     574978     902718     574978     902718     574978     902718     574978     902718     574978     902718     574978     902718     574938     281550     581756     736364     754432     177509     336819     557541     347365     037242     176600     731084     452829     315754     046499     553657     081756     358228     987679     336216     59370
H $-0.468571$ $1.776865$ $-3.0$ H $-1.619953$ $0.468738$ $-3.5$ H $-1.992123$ $3.807263$ $-0.6$ H $2.412765$ $2.239853$ $1.7$ Compound <b>3d</b> , conformation F: $H$ $0.258023$ $-5.716988$ $-0.6566666666666666666666666666666666666$	32481     518876     518876     528696     711700     967341     725104     1025104     231519     902718     574978     062469     073938     281550     581756     736364     754432     177509     336819     557541     347365     037242     176600     731084     452829     315754     046499     553657     081756     358228     987679     336216     95370     383212
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32481     518876     518876     528696     711700     967341     725104     1025104     207393     902718     936216     953627     936216     95370     83212     98686
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32481     518876     518876     528696     711700     967341     725104     107206     231519     902718     936819     937242     9365754     936216     953627     936216     95370     9383212     98686<

0	-4 128858	2 380065	0 602478
0	3 388561	0 471752	-1 173804
0	3.300301	1 071055	-1.173004
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0.0	mound [741 conf	ormation P.	
	.pound [/u1], CONT(	O TOTTO	0 040045
H	-4.966196	-0./63//0	-2.342047
С	-4.032819	-0.765192	-1.787657
Ν	-1.638198	-0.760181	-0.356088
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Ĉ	-2 207207	-0 614988	0 276020
	_1 05/000		0.210920
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0	-0.211408	-1.256599	-3.588664
N	-1 725485	-0.200660	2 495865
± N	T . 120100	0.200000	2.1/0000

нинснснссннснняяоооосннн	$\begin{array}{c} -1.886390\\ 0.750037\\ 0.563652\\ -0.346583\\ -0.330142\\ 2.107879\\ 2.311337\\ 0.170501\\ 2.386387\\ 0.499633\\ 0.209482\\ 0.312710\\ 3.095434\\ 4.114961\\ 2.906114\\ 3.025517\\ 2.332984\\ 0.517243\\ 3.158964\\ 0.182171\\ 1.744708\\ 0.618563\\ 1.658131\\ 0.520829\\ -0.017034\end{array}$	$\begin{array}{c} -0.238547\\ -0.878282\\ -0.662646\\ 0.087881\\ 0.467392\\ -0.941660\\ -1.928135\\ 1.220627\\ 0.061289\\ -1.196081\\ -1.907755\\ -1.648660\\ -0.652425\\ -0.673807\\ 0.331897\\ -1.913690\\ -0.906846\\ 2.310271\\ -0.167363\\ 0.843324\\ 1.218892\\ 1.838291\\ 2.111037\\ 1.363638\\ 2.724285\end{array}$	3.498009 -1.562017 -0.593675 2.101664 1.084938 -2.045139 -2.474613 2.993479 -3.174782 2.234575 1.458117 3.211605 -0.905433 -1.297974 -0.468664 0.456098 2.143118 2.589094 -4.083816 4.279637 -2.990766 5.236713 5.040210 6.212112 5.169674
11 C c == -	nound [2].	2.127203	5.1090/4
С	pound <b>[21]:</b> 3.509916 3.062798 1.757978 1.694156 3.796506 3.140107 1.051771 4.865875 3.660285 0.881113 1.077965 -0.257896 -0.569110 -0.404954 -0.665238 -1.377913 -1.591524 -0.913938 -2.682365 -3.333100 -2.502473 -1.201074 -1.745094 -0.655853 -2.189834 -1.652051 -2.743732 -3.713392	$\begin{array}{c} -1.814597\\ -0.849613\\ 1.505191\\ -0.783394\\ 0.334997\\ 1.532569\\ 0.367239\\ 0.325197\\ 2.482082\\ -2.059454\\ 2.820702\\ 2.979878\\ 3.908497\\ -1.892293\\ -0.961013\\ -2.961715\\ -3.244237\\ -3.825891\\ -2.607620\\ -3.488826\\ -2.283576\\ 2.153719\\ 2.805053\\ 1.422749\\ 1.439093\\ 0.774264\\ 2.162522\\ -1.308100\end{array}$	-0.554814 -0.345554 0.172422 -0.079519 -0.325419 -0.055152 0.173490 -0.516581 -0.010816 -0.088936 0.477067 0.217799 0.480095 0.313580 0.607485 0.359074 1.399320 -0.127345 -0.355891 -0.355891 -0.383223 -1.384353 -0.528154 -1.223710 -1.122894 0.403493 1.081792 1.009790 0.486062
0	-3.409324 1.736684	0.453347 3.741857	-0.592307 0.953080
0 Com	1./30684 1.373712 pound <b>[2.1</b> :	-3.128625	-0.439879
H	7.630436	-2.024135	-0.769314
C	5.725550	1.132548	0.211182
C C	5.743089 7 833473	-1.086542	-0.391591
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Ν	3.637661	-2.234930	-0.701423

H	3.254321	-1.321650	-0.491537
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U U	-1.350779	1 617691	0.300004
п u	-2 59120	4.04/001 2.001122	1 163960
с 11	-0 757275	2 A05325	1.103000 0 851356
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0	_5 517/01	_3 /5/101	0.30/041
0	J.JI/491	J J LOU	0./5440/

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