Unequivocal Structure Confirmation of a Breitfussin Analog by Anisotropic NMR Measurements

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Supplemental Information

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Structures of two Breitfussin Analogs, Cephalandole A and Flavonol

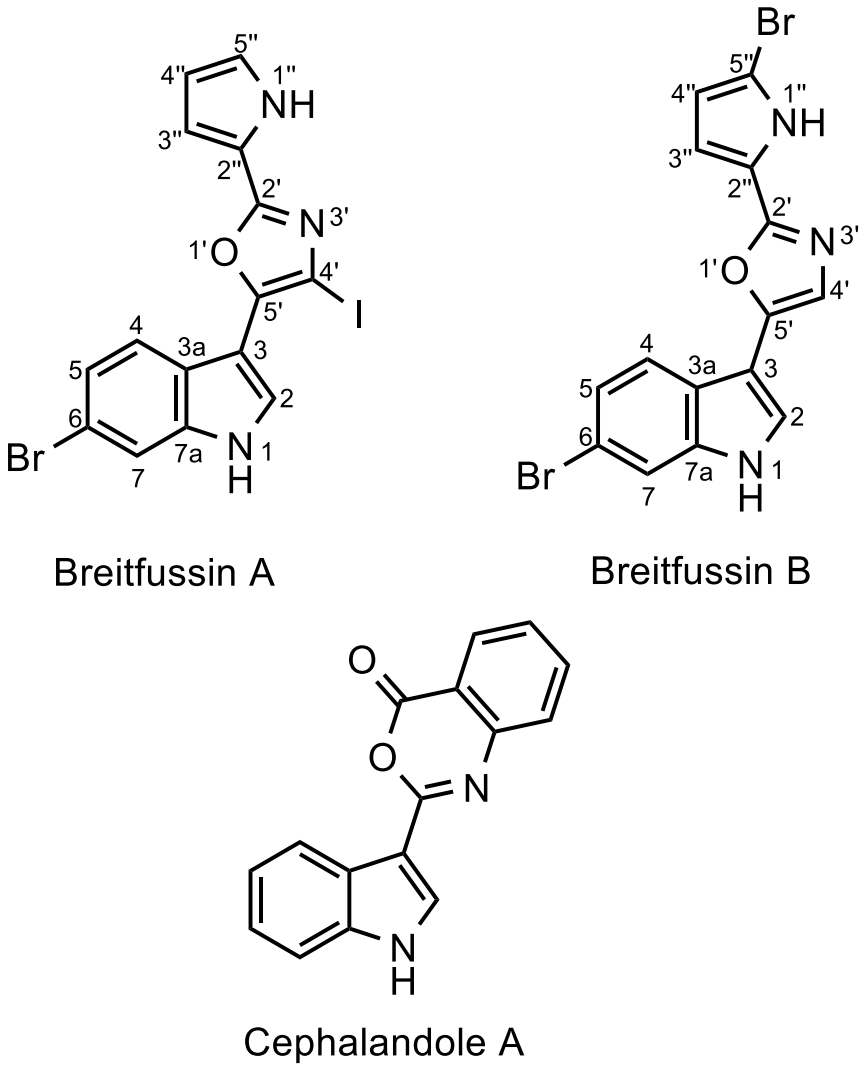

Figure S1. Structures of breitfussin A (4′-iodo analog), breitfussin B (desiodo-5″-bromo analog) and cephalandole A.

Experimental

2 mg of the breitfussin A analog sample was dissolved in 170 µL DMSO-d_6 solvent and following suite of experiments acquired on the sample: ^{1}H NMR experiment (12,019 Hz spectral width, 24,034 t1 points and 16 total scans); ^{13}C NMR experiment (29,762 Hz spectral width, 65,536 t1 points and 4096 total scans); COSY experiment (9014*8998 F1*F2 spectral width, 2048*256 t2*t1 points) with a total of 8 scans; HSQC experiment (9615*30171 F1*F2 spectral width, 2048*256 t2*t1 points) with a total of 48 scans; and an HMBC experiment optimized for 8 Hz (9615*30171 F1*F2 spectral width, 4096*256 t2*t1 points) with a total of 48 scans. All experiments were acquired with a Bruker Avance III 600 MHz spectrometer equipped with a 5 mm TXI cryogenic probe at a probe temperature of 25 °C.

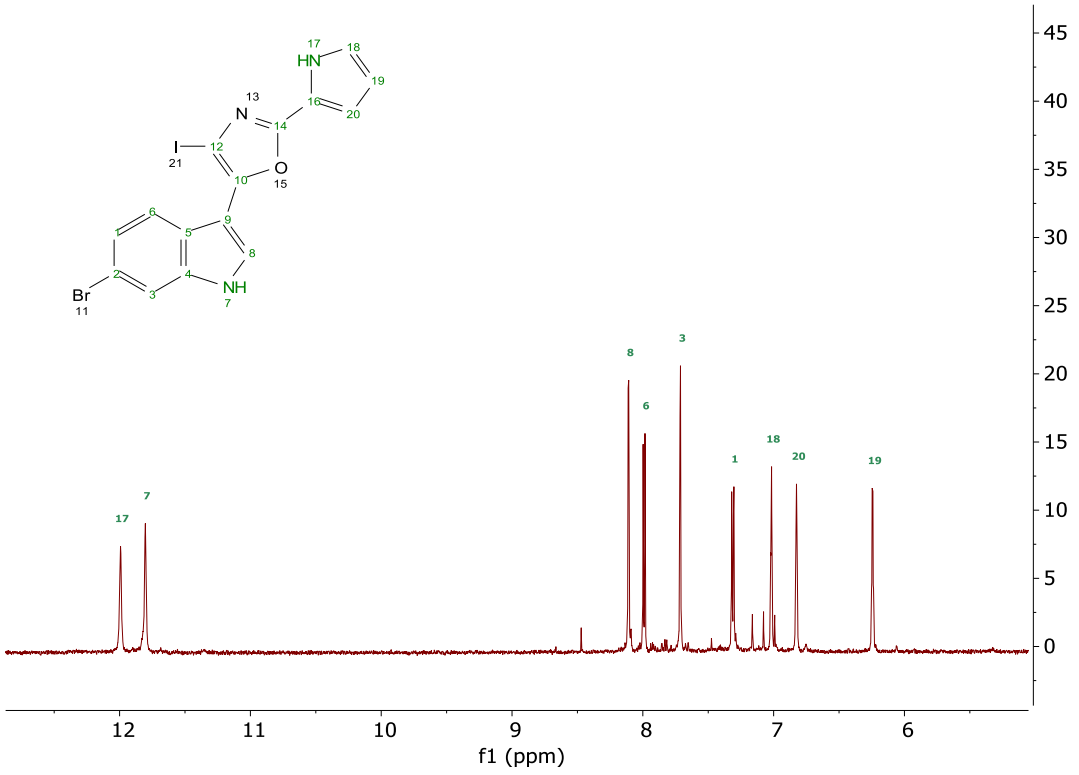

Figure S2. 600 MHz ^{1}H NMR spectrum of breitfussin A acquired with a 12,019 Hz spectral width and 24,034 t1 points and a total of 16 scans. Numbering scheme are shown inset.

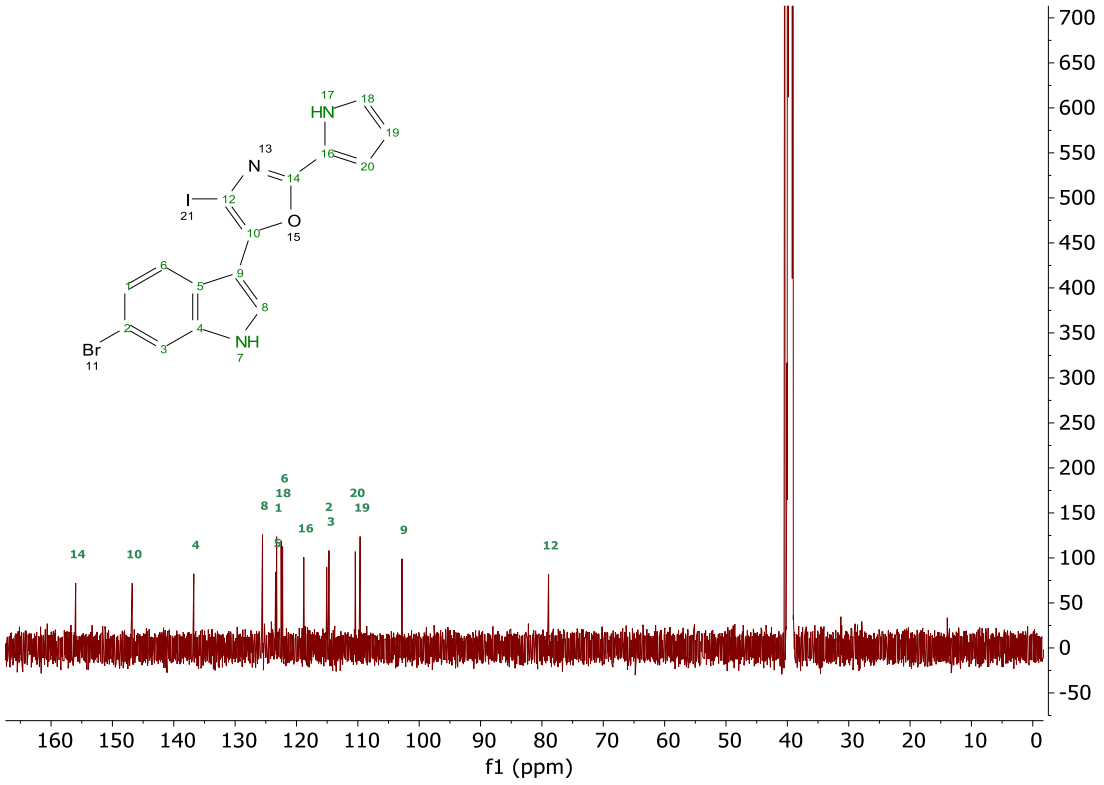

Figure S3: 150 MHz ^{13}C NMR spectrum of breitfussin A acquired with a 39,682 Hz spectral width, 131,072 t1 points and a total of 1,024 scans. See inset **Figure S2** for numbering scheme.

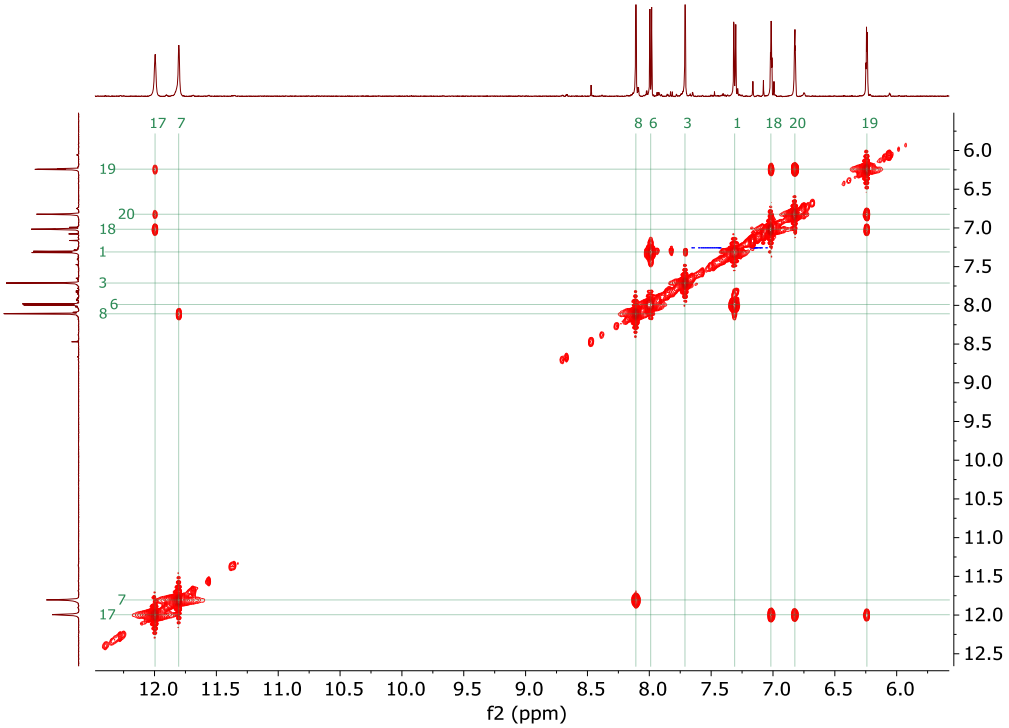

Figure S4: COSY spectrum showing correlations between vicinal protons of breitfussin A. See inset **Figure S2** for numbering scheme.

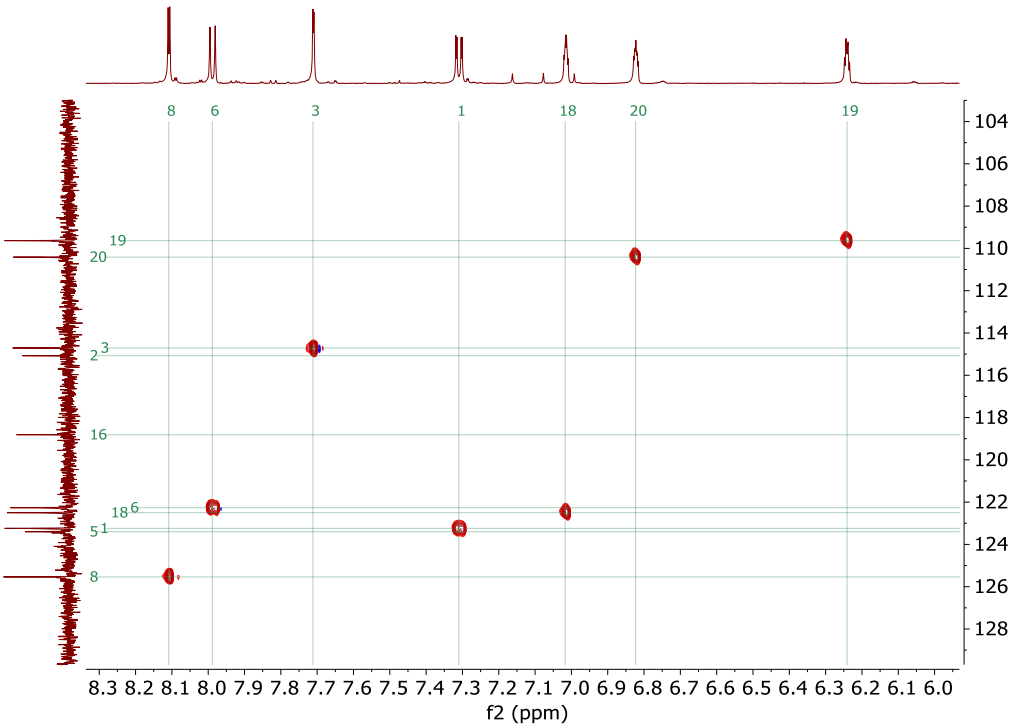

Figure S5: HSQC spectrum of breitfussin A showing protonated carbon resonance correlations. Since all protonated carbons in the molecule were methine resonances, multiplicity-editing was not employed. See inset **Figure S2** for numbering scheme.

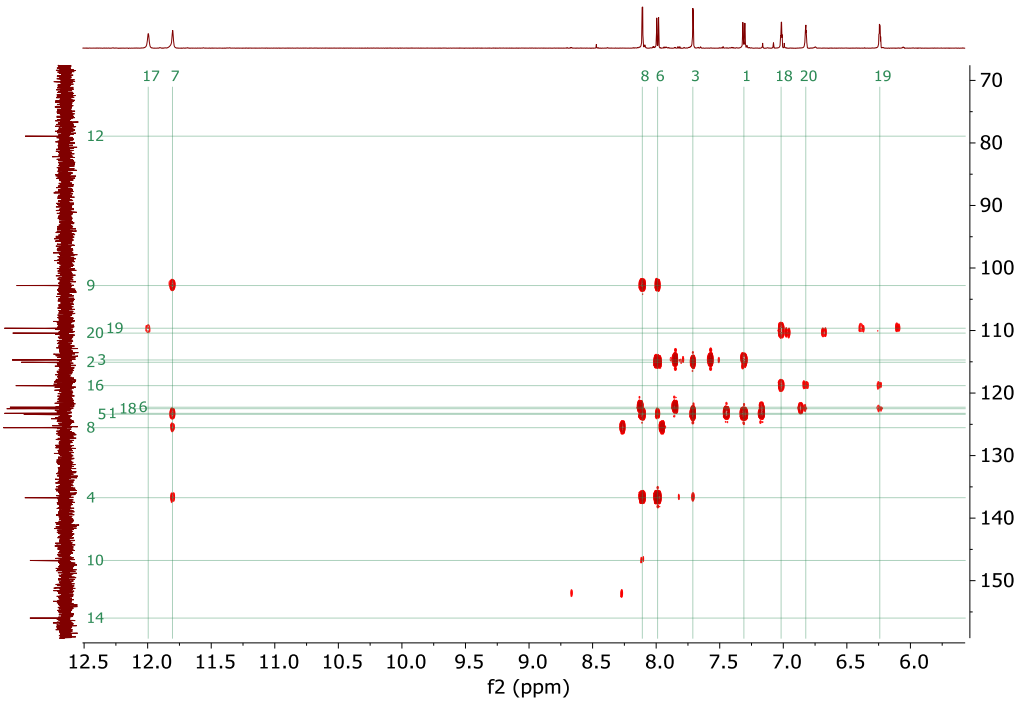

Figure S6: HMBC spectrum of breitfussin A analog optimized for 8 Hz. Pivotal correlation to the iodo-bearing carbon, C12, is too weak to be considered real a real correlation in the spectrum. See inset **Figure S2** for numbering scheme.

Poly-HEMA/MMA Co-polymer Gel Preparation

In this work, we adopted an in-house developed dimethyl sulfoxide (DMSO) compatible co-polymer gel of 2-hydroxyethyl methacrylate(HEMA) and methyl methacrylate (MMA) at 0.02% cross-linking ratio, that is a modification of the poly-HEMA gel first reported by Gil, *et al*.[1] This gel will be referred to as the poly-HEMA/MMA gel. The poly-HEMA/MMA gel consists of 35% HEMA (v/v), 35% MMA (v/v) and 30% methanol (v/v). The 0.02% gel cross-linking ratio was achieved with the addition of 20 µL per ml of a 1% ethylene glycol dimethacrylate (EDGMA) solution (prepared in MMA). 10 µL per ml of 6% V-70 (2,2′-azobis(2,4-dimethyl-4-methoxyvaleronitrile)) solution in acetone is added as the polymerization initiator (NOTE: HEMA, MMA and EDGMA reagents were filtered through basic alumina to remove polymerization inhibitors prior to use). The gel solution was properly mixed by vortexing to ensure homogeneity after which a very slow stream of nitrogen gas (to avoid spilling) was bubbled through the mixtures for a few seconds. The gel solution was then transferred into a 1/8" ID FEP (fluorinated ethylene propylene) tubing (Cole-Parmer catalog no.: EW-06450-05) – cut into 30 cm segments with one end sealed with a micro-stopper – using glass pipettes. The open end was then sealed with a micro-stopper and the gel was allowed to polymerize overnight in the oven at 50° C. The polymerized gel was then cut into 2.3 cm segments while inside the FEP tubing after which the cut gels were cured in the oven at 65° C for ~ 5hrs. The gels can now be easily pushed out from the FEP tubing. The cured gels are further cut into 2 cm gel sticks. The gels are washed by transferring into a glass vial filled with methanol and allowed to sit in the solvent for at least 4 hrs. The washing step is repeated 4 to 5 times by decanting the used solvent and replacing with fresh solvent. The washed gels are then dried on a glass surface inside the hood overnight, after which they were ready for use.

Gel sample preparation and data acquisition

Approximately 2 mg of breitfussin A was dissolved in 330 µL of DMSO-d_6 contained in a 4 ml vial with 5 µL of TMS added as reference. The pre-washed poly-HEMA/MMA gel (0.02 % cross-linking) gel stick was introduced into the vial containing the solution and allowed to incubate and equilibrate for two (2) days. Anisotropic NMR data, including *J*-modulated HSQC and ^{13}C NMR, were acquired utilizing a 4.2/3.0 mm stretching device (denoted here as isotropic and anisotropic ends, respectively) as described in the report by Liu, *et al*.[2] The "isotropic" *J*-modulated HSQC experiment (**Figure S7**) – gel in the 4.2 mm end – was acquired with a 4,795 *10,107 Hz F2*F1 spectral width and 1558*1000 t2*t1 points at 8 scans per increment. The "anisotropic" *J*-modulated HSQC experiment (**Figure S8**) – gel stretched in the 3.0 mm end – was acquired with a 3,000*10,560 Hz F2*F1 spectral width and 748*1000 t2*t1 points at 4 scans per increment. In the same vein, isotropic and anisotropic ^{13}C NMR experiments were acquired with 36,232 Hz spectral width, 144,912 t1 points and a total of 9,351 scans

(isotropic data) or 14,198 scans (anisotropic). Residual Dipolar Coupling (RDC) is the difference in the coupling constants measured between the two alignment conditions. Residual Chemical Shift Anisotropy (RCSA) is the difference in the chemical shifts between the two alignment conditions. The results obtained are summarized in **Table S1.**

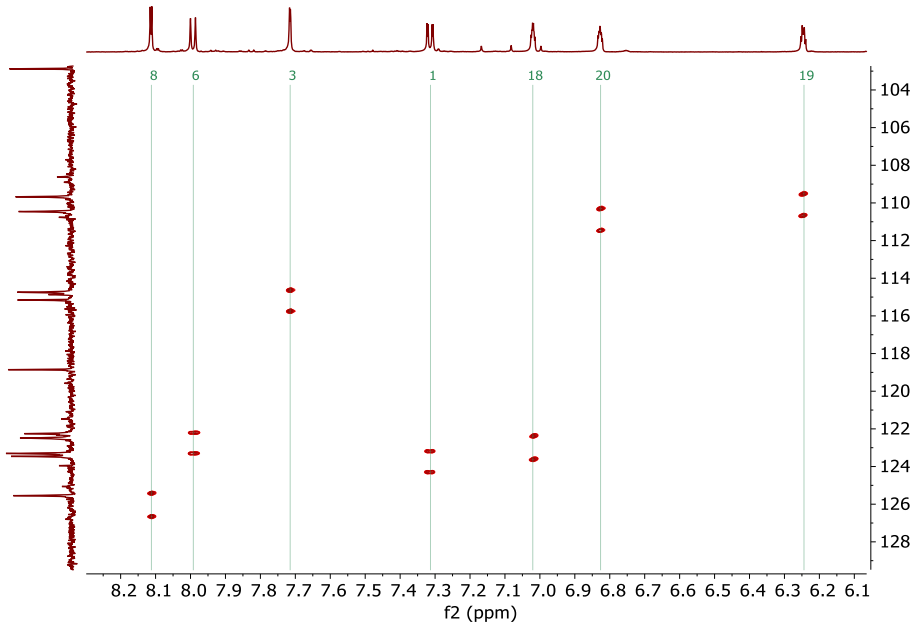

Figure S7: *J*-Modulated HSQC spectrum acquired with 4,795 *10,107 Hz F2*F1 spectral width (1558*1000 t2*t1 points) in the 4.2 mm end of the stretching device.[3] $^{1}J_{CH}$ values are measured as peak splitting in the indirect F1 dimension. ^{1}H and ^{13}C NMR spectra are shown as horizontal and vertical traces. See inset **Figure S2** for numbering scheme.

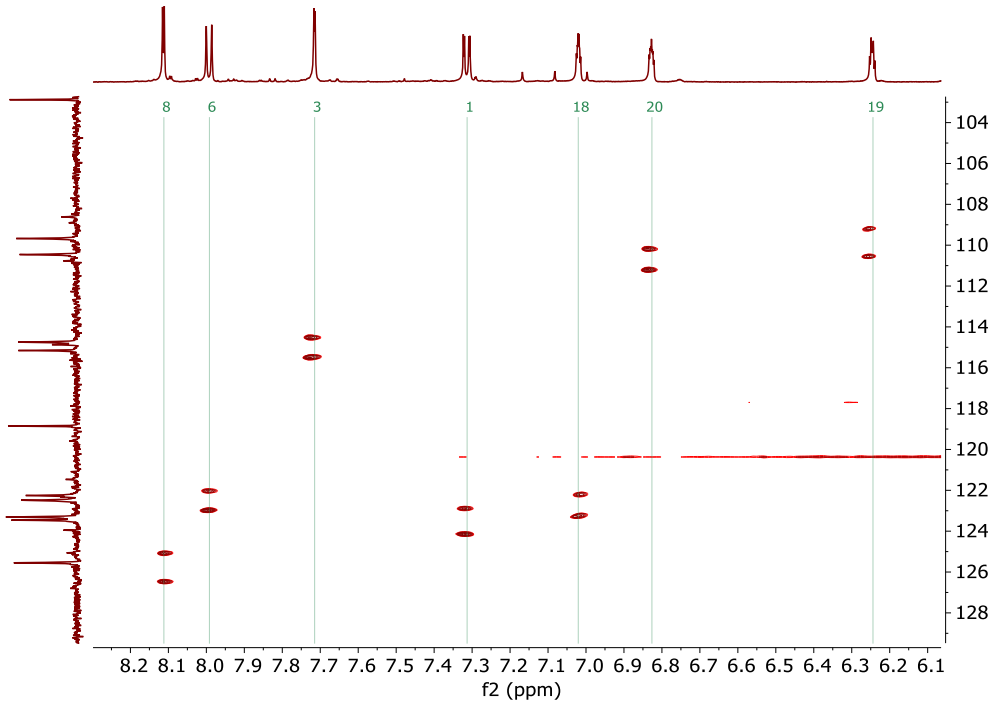

Figure S8: *J*-Modulated HSQC spectrum acquired with 3,000*10,560 Hz F2*F1 spectral width (748*1000 t2*t1 points) in the 3.0 mm end of the stretching device.[3] $^{1}J_{CH}$ values are measured as peak splitting in the indirect F1 dimension. ^{1}H and ^{13}C NMR spectra are shown as horizontal and vertical traces. See inset **Figure S2** for numbering scheme.

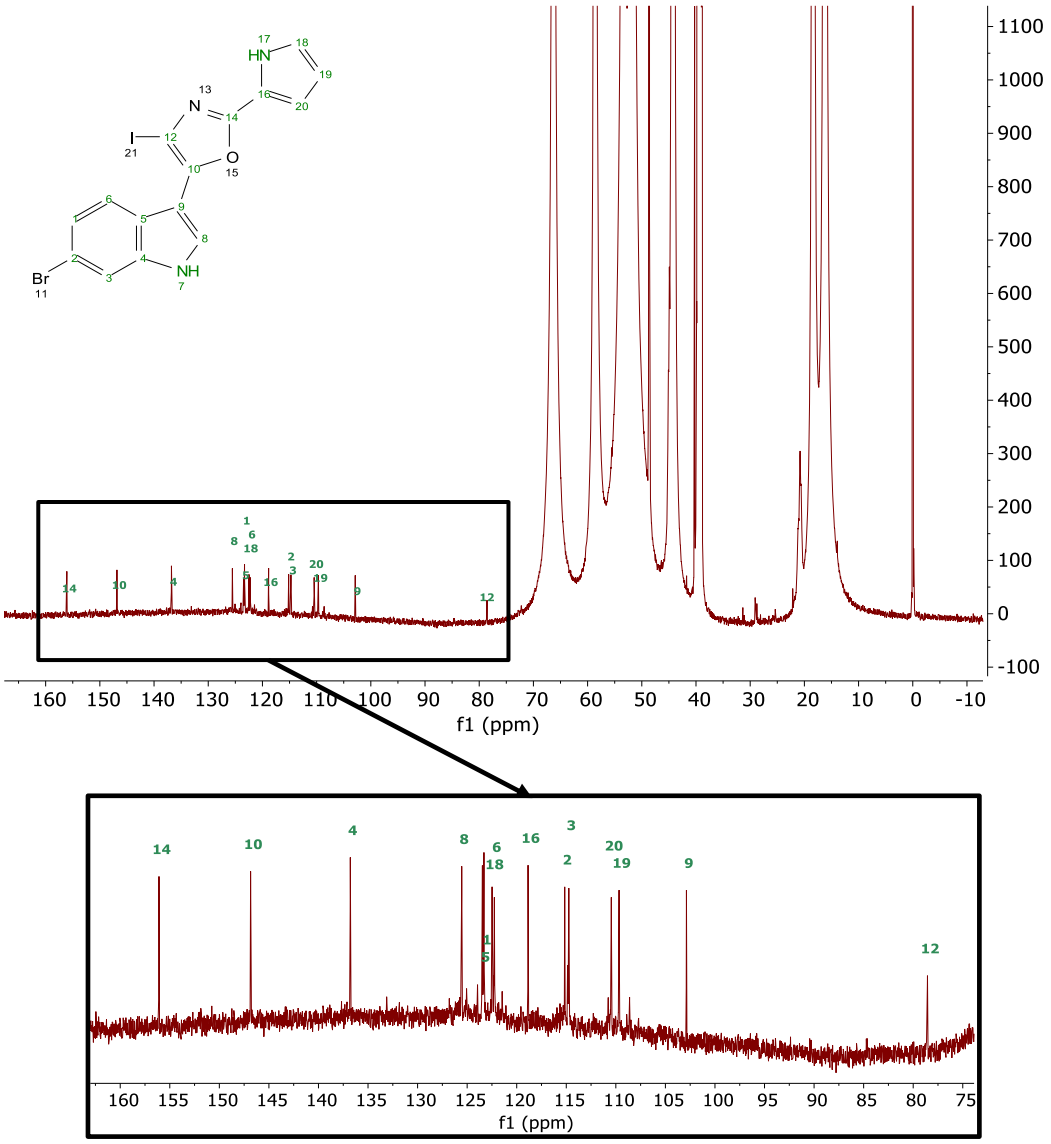

Figure S9: Isotropic ^{13}C NMR experiment acquired with 36,232 Hz spectral width, 144,912 t1 points and a total of 9,351 scans. See inset **Figure S2** for numbering scheme.

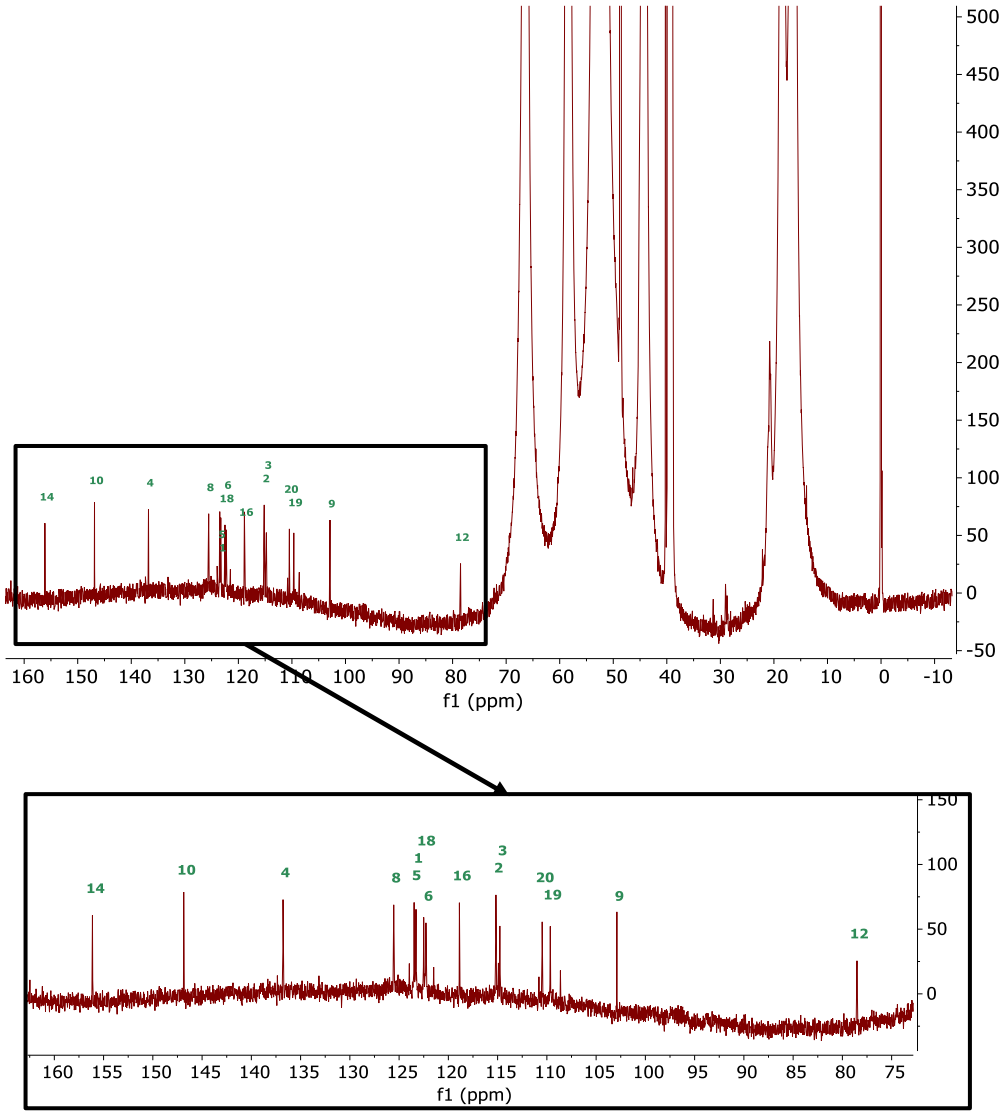

Figure S10: Anisotropic ^{13}C NMR experiment acquired with 36,232 Hz spectral width, 144,912 t1 points and a total of 14,198 scans. See inset **Figure S2** for numbering scheme.

Table S1: RDCs, RCSAs and Residual Quadrupolar Coupling (RQC) measured for breitfussin A acquired in the poly-HEMA/MMA gel with a 0.02 % cross-linking ratio, utilizing the stretching device (4.2/3.0 mm tube).[3] See corresponding atom numbering inset **Figure S9** (parenthetical carbon resonance number see structure in **Figure S1**).

Atom*	No. of Protons	RDC (Hz)	RCSA (Hz)
1 (C5)	1	25.01	-3.4
2 (C6)	-	-	2.3
3 (C7)	1	-24.53	4.5
4 (C7a)	-	-	-1.1
5 (C3a)	-	-	2.1
6 (C4)	1	-22.58	3.0
8 (C2)	1	23.69	-0.2
9 (C3)	-	-	2.4
10 (C5')	-	-	2.5
12 (C4')	-	-	-6.5
14 (C2')	-	-	6.1
16 (C2'')	-	-	3.3
18 (C5'')	1	-29.02	2.6
19 (C4'')	1	31.28	-3.2
20 (C3'')	1	-17.83	2.5
RQC		14.4	
*DFT atom numbering for Breitfussin A analog structure **1** used			

Breitfussin A Analog Solution Conformation Determined by NOESY NMR

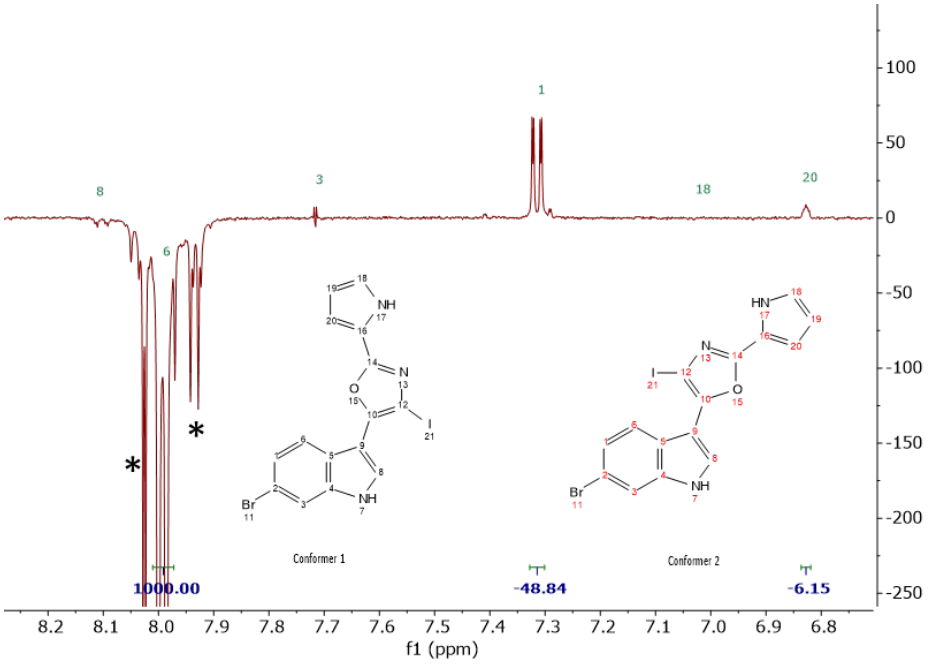

Figure S11. 1D selective ROESY experiment showing (inset), the two breitfussin A conformers whose relative populations were determined utilizing PANIC[2] corrected NOEs; H6 – H20 (6.15) and referenced to H6 – H1 (48.84). Signals from impurities are indicated with *.

The solution conformer population of the breitfussin analog was determined from ROESY data as shown below:

$$\frac{k}{r_{conf1}^6} + \frac{(1-k)}{r_{conf2}^6} = \frac{1}{r_{obs}^6}$$

Where *k* corresponds to the population of conformer 1. Solving for *k*,

$$k = \frac{(r_{conf1}^6 * r_{conf2}^6) - (r_{conf1}^6 * r_{obs}^6)}{r_{obs}^6 * (r_{conf2}^6 - r_{conf1}^6)}$$

The measured distances between H6 – H20 utilizing Density Functional Theory (DFT) geometries for conformers 1 and 2 are giving,

$r_{conf1} = 3.1$ Å and $r_{conf2} = 6.9$ Å

The calculated distance, r_{obs}, is given by

$$r_{obs} = r_{ref} * \left[\frac{ROE_{obs}}{ROE_{ref}}\right]^{-\frac{1}{6}}$$

Using the H1-H6 ROE signal as the reference,

$$r_{ref} = 2.5 \text{ Å}, ROE_{ref} = 48.84, ROE_{obs} = 6.15$$

$$r_{obs} = 3.567 \text{ Å}$$

Thus, substituting the values into:

$$k = \frac{(r_{conf1}^6 * r_{conf2}^6) - (r_{conf1}^6 * r_{obs}^6)}{r_{obs}^6 * (r_{conf2}^6 - r_{conf1}^6)}$$

The ROE derived population of conformer 1 is,

$$k = 0.454 \; or \; 45.4 \; \%$$

Isomeric breitfussin A analogs

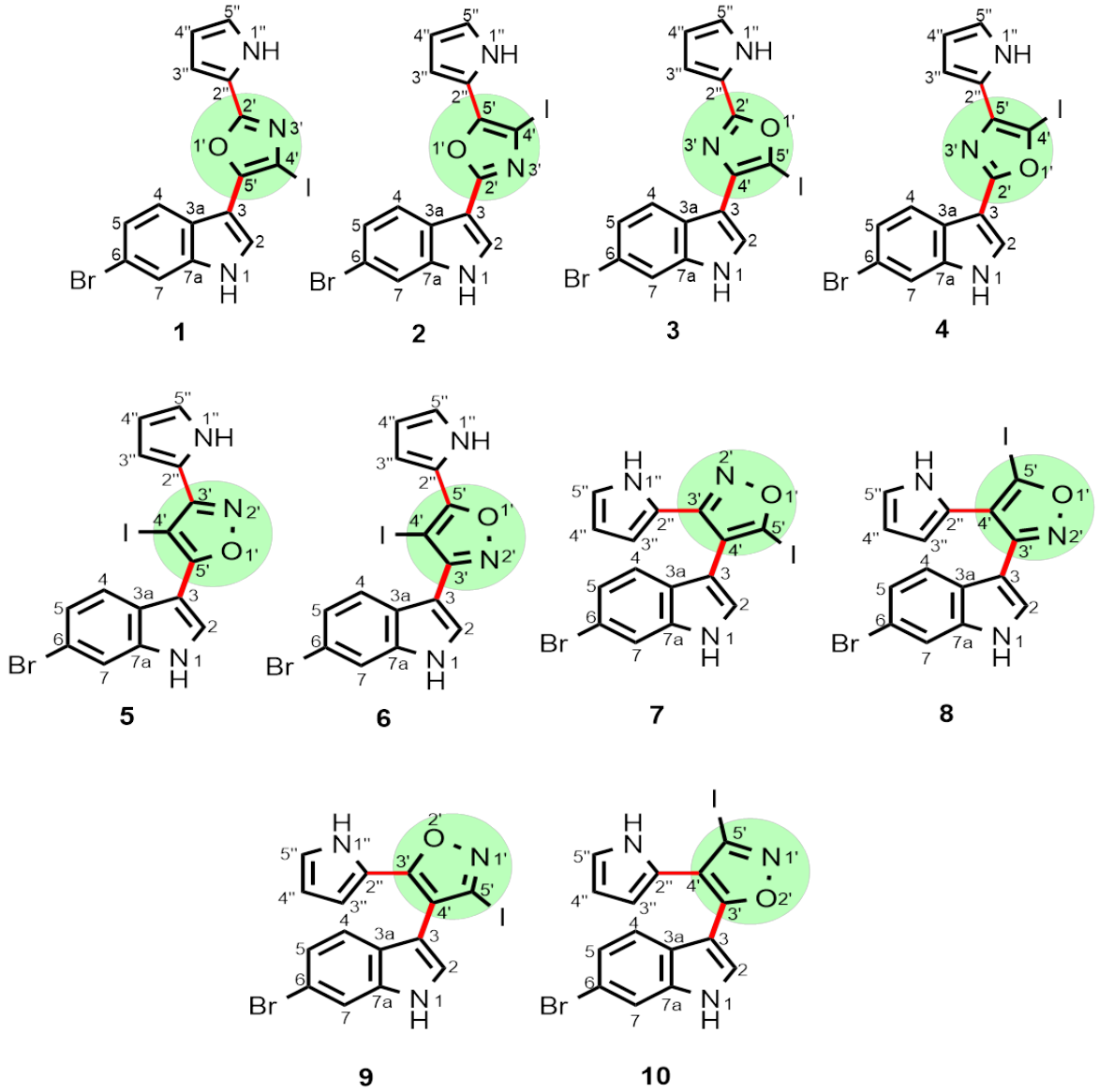

Figure S12. Ten possible isomeric breitfussin A analogs, based on the positional isomerism of the central ring (indicated with green circles), investigated in this work.

The ten isomeric breitfussin A analogs analysed in this work – involving the positional isomerism of the central oxazole or isoxazole ring – are shown in **Figure S12**. Four conformers were determined for each isomer, resulting from free rotation of the single bonds highlighted in red. The conformers generated preferentially adopt planar structures, in most cases after DFT optimization, with only a few off-plane stable conformations.

Chemical Shift Analysis of Isomeric Breitfussin A Analogs

Plots of chemical shift absolute errors of the non-halogenated carbons of ten isomeric breitfussin A analog are shown in **Figure S13**. Chemical shift values for the ten isomers were calculated by DFT methods using the model chemistry described in the section "DFT Geometry Optimizations and NMR Chemical Shift Calculations" (page S15). The theoretically determined chemical shift values were compared to experimentally measured values, which are tabulated in Table S2 below. The Mean Absolute Errors (MAE) were determined as 1.91, 3.83, 2.95, 4.21, 3.53, 3.46, 6.70, 4.33, 4.05 and 4.73 ppm, respectively, for isomers **1, 2, 3, 4, 5, 6, 7, 8, 9** and **10** (**Figure S13**). Although the MAE values favour the correct stereo-isomer, **1**, unequivocal isomeric differentiation is not feasible – especially to isomer **3** – due to inherent errors from theoretical calculations.

Table S2. ^{1}H and ^{13}C NMR chemical shifts of brietfussin A utilized in this study (parenthetical carbon resonance number see structure in **Figure S1**).

Chemical Shift Values (ppm)		
DFT Atom numbering (*)	**^{1}H Chemical shifts**	**^{13}C Chemical shifts**
1 (C5)	7.31	123.2
2 (C6)	-	115.1
3 (C7)	7.71	114.7
4 (C7a)	-	136.7
5 (C3a)	-	123.4
6 (C4)	7.99	122.3
8 (C2)	8.11	125.5
9 (C3)	-	102.8
10 (C5')	-	146.8
12 (C4')	-	78.9
14 (C2')	-	156.0
16 (C2'')	-	118.8
18 (C5'')	7.02	122.5
19 (C4'')	6.24	109.6
20 (C3'')	6.82	110.4
* Standardized carbon numbering as shown in **Figure S12**.		

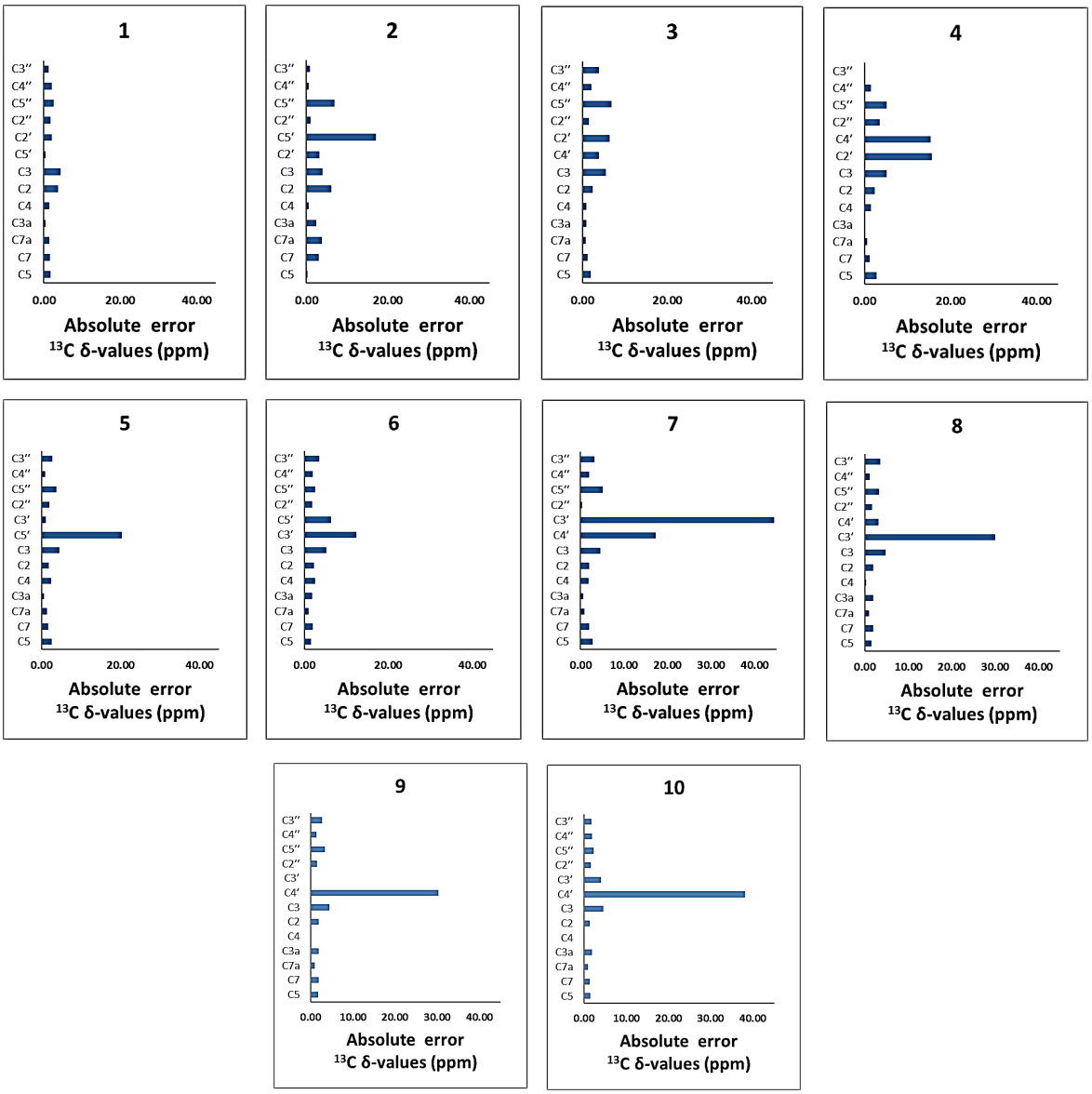

Figure S13. Bar charts of absolute errors of DFT-derived chemical shift values for the non-halogenated carbons, compared to experimentally measured data for isomeric structures **1, 2, 3, 4, 5, 6, 7, 8, 9** and **10** (see Figure S12). The Mean Absolute Error (MAE) of ^{13}C chemical shift is 1.91, 3.83, 2.95, 4.21, 3.53, 3.46, 6.70, 4.33, 4.05 and 4.73 ppm, respectively, **1, 2, 3, 4, 5, 6, 7, 8, 9** and **10** breitfussin A isomers.

Singular Value Decomposition (SVD) Analysis of Breitfussin A Analog

SVD analysis of the ten isomeric breitfussin structures cannot be unequivocally differentiated via the traditional approach that requires the computation of five free variables (Method A in **Table S3**). Isomers **1**, **2**, **4** and **7** yield low Q-values, which does not exclude the incorrect diastereomers as plausible structure for the breitfussin A analog investigated. On the other hand, enforcing additional constraints based on the planarity of the conformations adopted by the breitfussin isomers (Method B, discussed in main text and **Table S3**) allows unambiguous diastereomeric differentiation of the isomers.

Table S3. Single-tensor SVD analysis (variable weight) of the ten isomeric breitfussin A analog, utilizing the traditional method (A) and the modified method (B) as described in the main texts.

***Q*-factors from SVD analysis**		
Isomer	**Method A**	**Method B**
1	0.050	0.053
2	0.078	0.095
3	0.154	0.232
4	0.067	0.126
5	0.160	0.308
6	0.203	0.338
7	0.084	0.449
8	0.191	0.279
9	0.090	0.446
10	0.091	0.285

DFT Geometry Optimizations and NMR Calculations

All of the DFT calculations were performed using *Gaussian 16*, Revision B.01.5[5] Geometry optimizations and frequency calculations of **1**, **2**, **3**, **4**, **5**, **6**, **7**, **8**, **9** and **10** were performed using the M06-2X functional and the 6-31+G(d,p) basis set for C, H, N, and O, and the TZP-DKH basis set[6,7] for Br and I[8,9] using 'tight' geometry convergence criteria, the 'ultrafine' integration grid, and the SMD solvation model with DMSO as solvent and the keyword nosymmcav. All of the computations were performed in the input orientation through the use of the nosymm keyword. NMR shielding tensors and magnetic susceptibilities were calculated using the GIAO method on the optimized geometries with the mPW1PW91 density functional and the 6-311+G(2d,p) basis set for C, H, N, and O and TZP-DKH basis set for Br and I.

The basis functions utilized for bromine (Br) and iodine (I) (TZP-DKH basis set) are shown below:[5,6]

Br 0

S 7 1.00

1891721.28453019 0.0019998

299876.69022932 0.0055058

73577.47723328 0.0143340

22821.38425143 0.0343970

8196.66148892 0.0844542

3042.20569848 0.2335931

1114.04711267 0.6257158

S 2 1.00

27.88308617 -0.5952086

12.56697986 -0.4047913

S 1 1.00

416.79690877 1.0000000

S 1 1.00

162.83699705 1.0000000

S 1 1.00

60.95282138 1.0000000

S 1 1.00

4.29335357 1.0000000

S 1 1.00

1.86285469 1.0000000

S 1 1.00

0.43306174 1.0000000

S 1 1.00

0.1612887 1.0000000

P 7 1.00

9319.75302208 0.0007979

2376.91773965 0.0034677

850.05093709 0.0139712

333.27682069 0.0543097

133.67709985 0.1755638

55.61145698 0.3693407

24.09110501 0.3825488

P 2 1.00

4.59144998 -0.5931901

2.01522298 -0.4068098

P 1 1.00

10.32325402 1.0000000

P 1 1.00

0.74175022 1.0000000

P 1 1.00

0.29419421 1.0000000

P 1 1.00

0.10541093 1.0000000

D 4 1.00

168.94701922 0.0133602

49.42559982 0.0911855

17.8625704 0.3148117

7.02094166 0.5806425

D 1 1.00

2.76152556 1.0000000

D 1 1.00

1.0146000 1.0000000

F 1 1.00

10.92125998 1.0000000

F 1 1.00

3.0839599 1.0000000

G 1 1.00

8.36545878 1.0000000

****

I 0

S 8 1.00

5464702.08060097 0.0022010

849942.52168504 0.0059336

207458.86762606 0.0137360

64929.86485391 0.0289591

23909.80880875 0.0599806

9850.71275593 0.1154691

4222.34623514 0.2554331

1781.76403452 0.5182871

S 2 1.00

749.21394356 -0.5544582

318.75246448 -0.4455417

S 2 1.00

59.88344918 -0.6579130

29.50227605 -0.3420869

S 2 1.00

12.24593624 -0.6349870

6.20345391 -0.3650129

S 2 1.00

2.43764323 0.6518901

1.14985168 0.3481098

S 1 1.00

118.02205930 1.0000000

S 1 1.00

0.30638210 1.0000000

S 1 1.00

0.11926836 1.0000000

S 1 1.00

0.05963418 1.0000000

P 7 1.00

20182.20166081 0.0016094

4999.21100888 0.0059094

1768.53795847 0.0204900

734.7752808 0.0629189

317.5116541 0.1798365

139.60118455 0.3605064

63.12833732 0.3687292

P 2 1.00

13.45203045 -0.6684080

6.52579989 -0.3315919

P 3 1.00

3.02467901 0.6059378

1.38040546 0.3385645

0.52669045 0.0554975

P 1 1.00

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P 1 1.00

0.22217820 1.0000000

P 1 1.00

0.08328104 1.0000000

P 1 1.00

0.04164052 1.0000000

D 6 1.00

565.9883795 0.0066068

168.69681731 0.0466142

63.14306896 0.1755992

26.1030685 0.3583238

11.24530421 0.3404563

4.6390732 0.0723995

D 1 1.00

1.91572411 1.0000000

D 1 1.00

0.72024616 1.0000000

D 1 1.00

0.36012308 1.0000000

F 1 1.00

3.85297909 1.0000000

F 1 1.00

1.265860195 1.0000000

G 1 1.00

2.97888999 1.0000000

Other model chemistries explored in geometry optimizations and frequencies (Table 1 in main text) include (1) the B3LYP density functional and the 6-31G* basis set for C, H, N, O, and Br, and MIDI! for I, and (2) the M06-2X density functional and the 6-31+G** basis set for C, H, N, O, and Br, and DGDZVP for I. Single-point energies incorporating the second-order Douglas-Kroll-Hess relativistic corrections were additionally evaluated using these two model chemistries on the corresponding optimized geometries.

Table S4. The DFT SCF energies of conformers of the isomeric breitfussin A analogs calculated with the M06-2X functional and the TZP-DKH basis set for I and Br and the 6-31+G(d,p) for the other elements.

DFT SCF energies				
Isomer	**Conformer 1**	**Conformer 2**	**Conformer 3**	**Conformer 4**
1	-10227.3272747	-10227.3269343	-10227.3257936	-10227.3255345
2	-10227.3280597	-10227.3266542	-10227.3280581	-10227.3292980
3	-10227.3225896	-10227.3226754	-10227.3210185	-10227.3211404
4	-10227.3249022	-10227.3253170	-10227.3244017	-10227.3251064
5	-10227.2863312	-10227.2854944	-10227.2857097	-10227.2851302
6	-10227.2854817	-10227.2860022	-10227.2864821	-10227.2866630
7	-10227.2815953	-10227.2820551	-10227.2810071	-10227.2818050
8	-10227.2783665	-10227.2776143	-10227.2784319	-10227.2776464
9	-10227.2816221	-10227.2820903	-10227.2809589	-10227.2818283
10	-10227.2823324	-10227.2818157	-10227.2819784	-10227.2820598

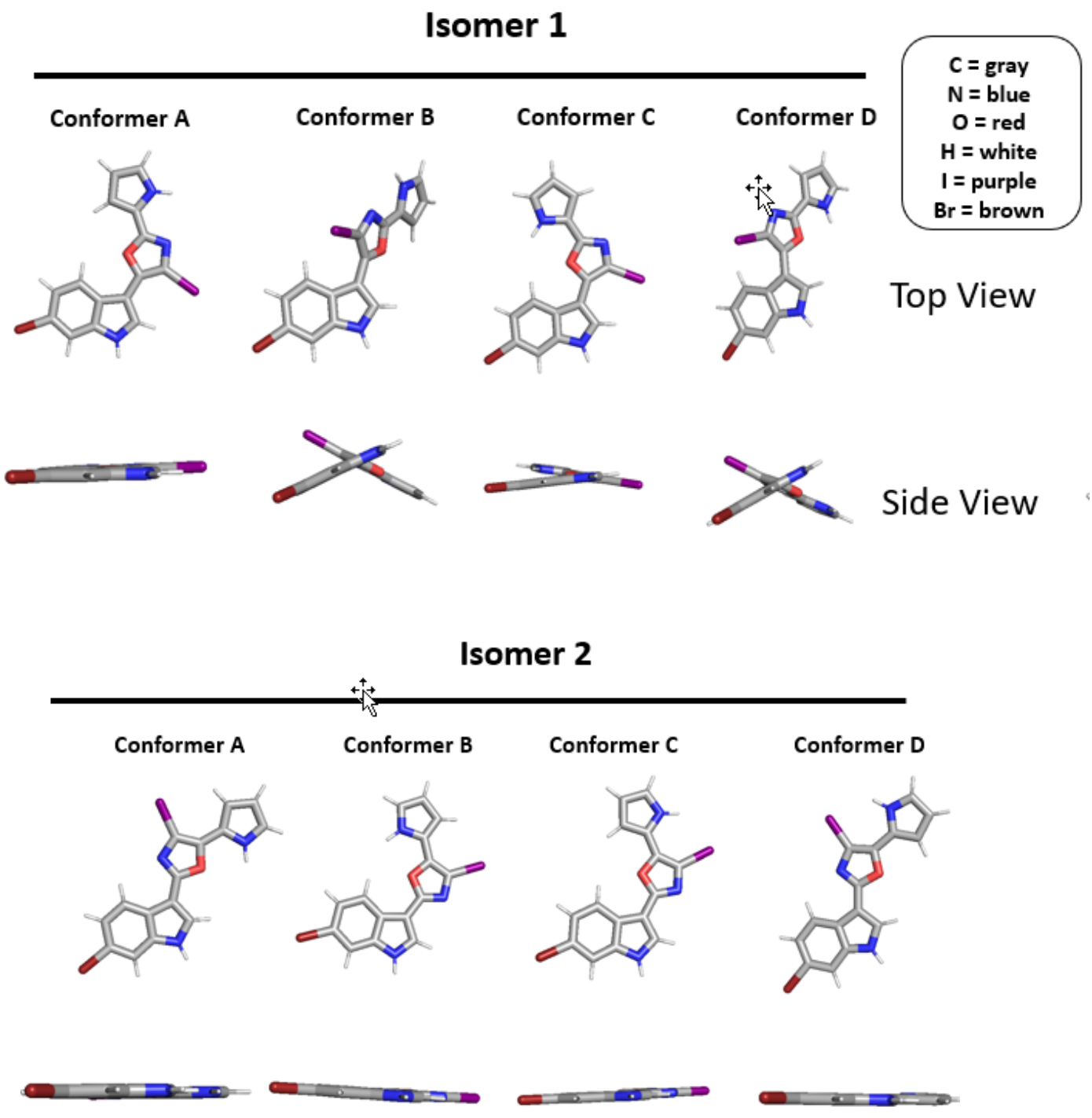

Figure S14. Top and side views of the four conformers of isomeric breitfussin A structures, **1**-**2**.

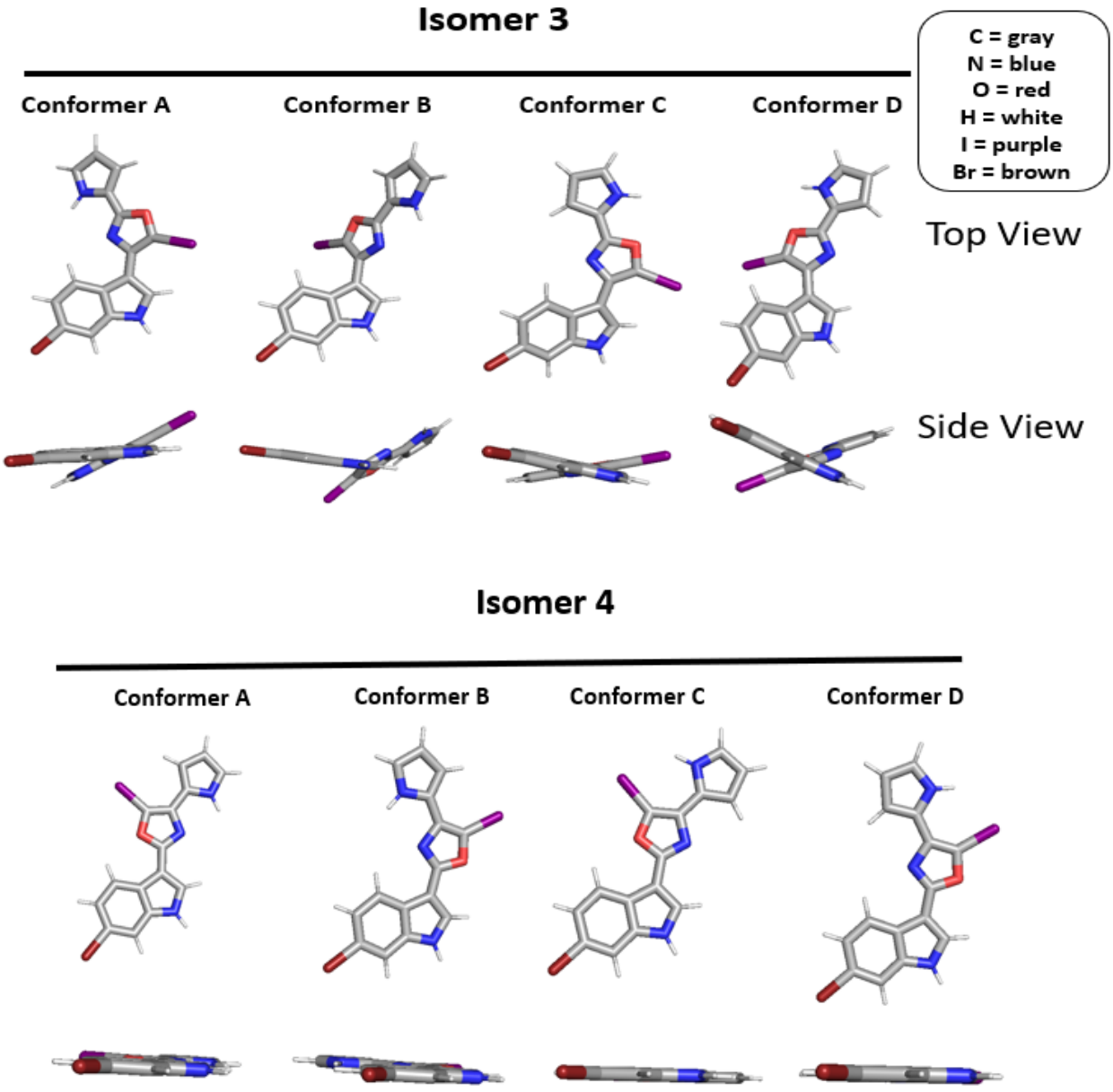

Figure S15. Top and side views of the four conformers of isomeric breitfussin A structures, **3**-**4**.

Table S5. Absolute value of biaryl dihedral angle between the oxazole and indole ring (degree of planarity estimate) for the different conformations of **1**-**4**. (See **Figure S14** and **Figure S15** above).

Conformer	Isomer 1	Isomer 2	Isomer 3	Isomer 4
A	2.3°	0.0°	27.3°	0.0°
B	49.9°	0.0°	47.4°	0.0°
C	14.8°	0.0°	25.4°	0.0°
D	51.2°	0.0°	48.1°	0.0°

DFT Structures of the Ten Isomeric Breitfussin A Analogs

Breitfussin A analog Isomer 1												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	-3.318	-0.233	1.042	-4.056	-0.102	1.704	-3.208	-0.475	1.118	-4.24	-0.312	1.096
C2	-3.737	-0.83	2.245	-3.995	-0.108	3.112	-3.539	-0.859	2.431	-4.354	-0.476	2.491
C3	-2.858	-1.381	3.156	-2.822	0.079	3.818	-2.591	-1.185	3.38	-3.284	-0.348	3.356
C4	-1.501	-1.315	2.818	-1.671	0.296	3.05	-1.255	-1.112	2.967	-2.054	-0.026	2.769
C5	-1.032	-0.724	1.62	-1.694	0.335	1.637	-0.875	-0.728	1.658	-1.903	0.171	1.377
C6	-1.97	-0.178	0.726	-2.908	0.125	0.964	-1.879	-0.408	0.729	-3.017	0.017	0.536
N7	-0.41	-1.77	3.515	-0.369	0.475	3.45	-0.11	-1.378	3.675	-0.818	0.132	3.348
C8	0.729	-1.496	2.82	0.431	0.629	2.354	0.98	-1.183	2.878	0.106	0.422	2.386
C9	0.408	-0.851	1.641	-0.336	0.557	1.211	0.569	-0.783	1.623	-0.51	0.463	1.154
C10	1.329	-0.394	0.63	0.128	0.664	-0.157	1.416	-0.47	0.499	0.117	0.734	-0.123
Br11	-5.615	-0.878	2.632	-5.619	-0.409	4.088	-5.393	-0.931	2.917	-6.074	-0.917	3.215
C12	2.68	-0.368	0.45	-0.257	1.38	-1.245	2.721	-0.653	0.153	-0.143	1.574	-1.158
N13	2.997	0.209	-0.758	0.534	1.082	-2.33	2.981	-0.1	-1.08	0.778	1.411	-2.167
C14	1.845	0.517	-1.277	1.379	0.204	-1.87	1.84	0.396	-1.454	1.576	0.486	-1.716
O15	0.796	0.184	-0.495	1.194	-0.099	-0.57	0.85	0.21	-0.551	1.238	0.028	-0.491
C16	1.579	1.149	-2.544	2.446	-0.448	-2.586	1.519	1.091	-2.676	2.74	-0.072	-2.358
N17	2.604	1.513	-3.377	2.685	-0.152	-3.902	0.259	1.566	-2.936	3.496	-1.06	-1.779
C18	2.097	2.082	-4.504	3.732	-0.895	-4.354	0.244	2.177	-4.153	4.524	-1.391	-2.607
C19	0.717	2.087	-4.401	4.179	-1.687	-3.312	1.516	2.096	-4.691	4.433	-0.606	-3.743
C20	0.385	1.494	-3.156	3.365	-1.406	-2.187	2.328	1.407	-3.757	3.302	0.232	-3.587
I21	4.151	-1.057	1.703	-1.725	2.812	-1.35	4.206	-1.599	1.207	-1.616	3.001	-1.263
H22	-4.051	0.186	0.36	-5.003	-0.271	1.203	-3.993	-0.233	0.411	-5.112	-0.44	0.464
H23	-3.187	-1.839	4.082	-2.784	0.057	4.902	-2.853	-1.482	4.39	-3.381	-0.492	4.427

H24	-1.657	0.285	-0.203	-2.948	0.122	-0.121	-1.634	-0.113	-0.286	-2.923	0.133	-0.54
H25	-0.44	-2.234	4.415	-0.046	0.491	4.409	-0.073	-1.674	4.642	-0.617	0.047	4.337
H26	1.694	-1.78	3.214	1.495	0.788	2.462	1.978	-1.332	3.263	1.143	0.588	2.645
H27	3.589	1.377	-3.178	2.159	0.52	-4.449	-0.542	1.481	-2.322	3.324	-1.482	-0.874
H28	2.751	2.437	-5.287	4.075	-0.804	-5.375	-0.664	2.618	-4.538	5.234	-2.155	-2.326
H29	0.028	2.474	-5.138	5	-2.389	-3.357	1.824	2.49	-5.65	5.106	-0.635	-4.588
H30	-0.604	1.335	-2.748	3.431	-1.845	-1.201	3.377	1.164	-3.846	2.928	0.974	-4.28

Breitfussin A analog isomer 2												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	-2.018	0	-4.233	-0.739	-0.026	-3.433	-0.722	0	-3.502	-1.923	-0.013	-4.282
C2	-0.976	0	-5.179	0.213	-0.011	-4.47	0.241	0	-4.528	-0.871	-0.028	-5.217
C3	0.361	0	-4.828	1.575	0.007	-4.239	1.601	0	-4.283	0.462	-0.029	-4.852
C4	0.634	0	-3.456	1.97	0.009	-2.897	1.982	0	-2.937	0.721	-0.013	-3.477
C5	-0.382	0	-2.472	1.048	-0.006	-1.822	1.049	0	-1.872	-0.306	0.003	-2.504
C6	-1.726	0	-2.878	-0.327	-0.023	-2.11	-0.324	0	-2.174	-1.646	0.004	-2.924
N7	1.847	0	-2.806	3.237	0.023	-2.363	3.244	0	-2.389	1.926	-0.012	-2.815
C8	1.648	0	-1.46	3.165	0.018	-1.005	3.156	0	-1.032	1.713	0.002	-1.47
C9	0.293	0	-1.199	1.841	0.001	-0.617	1.828	0	-0.659	0.355	0.013	-1.224
C10	-0.335	0	0.096	1.385	-0.008	0.75	1.355	0	0.703	-0.281	0.029	0.067
Br11	-1.437	0	-7.041	-0.414	-0.018	-6.282	-0.366	0	-6.347	-1.311	-0.051	-7.084
O12	0.449	0	1.203	0.049	0	0.977	0.017	0	0.91	0.497	0.007	1.176
C13	-0.409	0	2.272	-0.104	-0.007	2.339	-0.156	0	2.268	-0.363	0.032	2.24
C14	-1.664	0	1.747	1.155	-0.019	2.855	1.096	0	2.802	-1.615	0.068	1.709
N15	-1.607	0	0.371	2.088	-0.021	1.845	2.046	0	1.806	-1.555	0.065	0.334
C16	0.173	0	3.59	-1.45	0	2.854	-1.511	0	2.757	0.223	0.011	3.557
N17	1.536	0	3.759	-2.529	0.044	2.005	-1.821	0	4.094	-0.528	-0.04	4.705
C18	1.838	0	5.089	-3.686	0.041	2.727	-3.175	0	4.253	0.293	-0.053	5.793
C19	0.651	0	5.796	-3.353	-0.007	4.066	-3.755	0	2.999	1.6	-0.007	5.345
C20	-0.407	0	4.851	-1.938	-0.032	4.153	-2.703	0	2.047	1.559	0.033	3.927
I21	-3.464	0	2.726	1.733	-0.031	4.821	1.641	0	4.78	-3.419	0.132	2.686
H22	-3.05	0	-4.566	-1.797	-0.04	-3.671	-1.777	0	-3.75	-2.952	-0.014	-4.626
H23	1.158	0	-5.564	2.304	0.019	-5.042	2.338	0	-5.078	1.267	-0.041	-5.578
H24	-2.528	0	-2.147	-1.068	-0.036	-1.318	-1.071	0	-1.388	-2.455	0.016	-2.202

H25	2.754	0	-3.256	4.098	0.036	-2.896	4.111	0	-2.913	2.838	-0.021	-3.255
H26	2.487	0	-0.777	4.059	0.028	-0.397	4.044	0	-0.415	2.544	0.005	-0.779
H27	2.218	0	3.011	-2.479	0.082	0.995	-1.145	0	4.848	-1.54	-0.079	4.741
H28	2.866	0	5.421	-4.646	0.072	2.231	-3.614	0	5.24	-0.116	-0.092	6.792
H29	0.555	0	6.873	-4.05	-0.022	4.893	-4.816	0	2.792	2.483	-0.002	5.968
H30	-1.466	0	5.059	-1.34	-0.07	5.051	-2.793	0	0.969	2.4	0.075	3.249

Breitfussin A analog isomer 3												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	3.124	1.952	0.222	4.379	0.49	-0.344	3.409	1.522	0.38	4.275	1.042	-0.38
C2	3.143	3.305	0.613	4.783	1.772	0.078	3.601	2.811	0.911	4.517	2.398	-0.082
C3	2.022	3.975	1.061	3.891	2.772	0.416	2.574	3.57	1.439	3.509	3.306	0.176
C4	0.837	3.231	1.109	2.533	2.45	0.301	1.302	2.984	1.417	2.201	2.809	0.109
C5	0.77	1.87	0.723	2.084	1.186	-0.149	1.062	1.692	0.888	1.912	1.462	-0.217
C6	1.94	1.233	0.275	3.03	0.195	-0.46	2.142	0.96	0.366	2.974	0.573	-0.451
N7	-0.418	3.612	1.512	1.423	3.204	0.592	0.104	3.479	1.867	1.008	3.444	0.346
C8	-1.276	2.553	1.4	0.295	2.471	0.347	-0.883	2.56	1.647	-0.021	2.558	0.185
C9	-0.597	1.454	0.92	0.644	1.225	-0.119	-0.35	1.44	1.047	0.478	1.327	-0.171
Br10	4.807	4.256	0.525	6.663	2.136	0.2	5.375	3.543	0.901	6.337	3.002	-0.016
C11	-1.14	0.133	0.655	-0.275	0.153	-0.483	-1.061	0.24	0.639	-0.304	0.124	-0.426
C12	-2.2	-0.519	1.203	-0.277	-0.647	-1.58	-2.222	-0.301	1.095	-0.216	-0.757	-1.456
O13	-2.329	-1.736	0.599	-1.321	-1.521	-1.485	-2.497	-1.424	0.367	-1.146	-1.739	-1.272
C14	-1.32	-1.78	-0.294	-1.926	-1.201	-0.322	-1.469	-1.526	-0.504	-1.776	-1.401	-0.124
N15	-0.584	-0.709	-0.307	-1.354	-0.222	0.314	-0.592	-0.574	-0.389	-1.322	-0.311	0.419
I16	-3.535	-0.085	2.681	0.827	-0.699	-3.293	-3.541	0.19	2.569	0.87	-0.806	-3.179
N17	-0.174	-3.065	-2.03	-3.735	-1.69	1.247	-2.465	-3.574	-1.453	-3.22	-3.386	-0.342
C18	-1.177	-2.966	-1.102	-3.09	-1.956	0.069	-1.466	-2.634	-1.427	-2.834	-2.263	0.344
C19	-1.911	-4.141	-1.135	-3.761	-2.989	-0.566	-0.54	-2.967	-2.403	-3.625	-2.158	1.476
C20	-1.318	-4.968	-2.121	-4.846	-3.349	0.271	-1.006	-4.148	-3.029	-4.515	-3.26	1.461
C21	-0.247	-4.271	-2.654	-4.8	-2.526	1.383	-2.199	-4.496	-2.418	-4.237	-4	0.324
H22	4.036	1.475	-0.119	5.124	-0.262	-0.578	4.253	0.97	-0.018	5.108	0.37	-0.554
H23	2.048	5.016	1.364	4.215	3.75	0.756	2.733	4.561	1.85	3.709	4.343	0.422
H24	1.923	0.191	-0.025	2.714	-0.794	-0.776	1.992	-0.033	-0.045	2.786	-0.474	-0.669

H25	-0.676	4.536	1.836	1.434	4.156	0.936	-0.034	4.388	2.291	0.902	4.418	0.601
H26	-2.32	2.662	1.659	-0.687	2.893	0.514	-1.906	2.774	1.921	-1.048	2.869	0.327
H27	0.514	-2.345	-2.218	-3.455	-0.98	1.913	-3.28	-3.587	-0.851	-2.813	-3.719	-1.207
H28	-2.77	-4.368	-0.517	-3.494	-3.425	-1.519	0.362	-2.413	-2.625	-3.558	-1.373	2.217
H29	-1.635	-5.96	-2.411	-5.579	-4.122	0.086	-0.528	-4.686	-3.836	-5.274	-3.491	2.196
H30	0.462	-4.54	-3.423	-5.438	-2.472	2.253	-2.873	-5.321	-2.595	-4.68	-4.907	-0.059

Breitfussin A analog isomer 4												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	1.959	0	-4.15	0.562	0	-3.732	1.868	0	-4.185	0.5	0	-3.822
C2	0.971	0	-5.152	-0.491	0	-4.666	0.873	0	-5.18	-0.578	0	-4.728
C3	-0.382	0	-4.873	-1.824	0	-4.299	-0.478	0	-4.892	-1.9	0	-4.325
C4	-0.73	0	-3.517	-2.081	0	-2.924	-0.816	0	-3.534	-2.12	0	-2.944
C5	0.23	0	-2.477	-1.054	0	-1.952	0.15	0	-2.5	-1.067	0	-1.999
C6	1.595	0	-2.813	0.286	0	-2.374	1.513	0	-2.845	0.26	0	-2.457
N7	-1.977	0	-2.938	-3.286	0	-2.26	-2.06	0	-2.946	-3.308	0	-2.249
C8	-1.855	0	-1.584	-3.072	0	-0.917	-1.929	0	-1.593	-3.058	0	-0.912
C9	-0.518	0	-1.244	-1.714	0	-0.671	-0.59	0	-1.262	-1.694	0	-0.702
C10	-0.009	0	0.104	-1.079	0	0.622	-0.072	0	0.084	-1.028	0	0.576
Br11	1.533	0	-6.985	-0.053	0	-6.533	1.423	0	-7.016	-0.19	0	-6.606
N12	-0.663	0	1.228	0.193	0	0.896	-0.722	0	1.21	0.249	0	0.821
C13	0.307	0	2.224	0.273	0	2.285	0.252	0	2.203	0.362	0	2.208
C14	1.524	0	1.621	-0.993	0	2.775	1.466	0	1.591	-0.895	0	2.724
O15	1.333	0	0.269	-1.864	0	1.723	1.272	0	0.24	-1.79	0	1.694
C16	-0.067	0	3.625	1.558	0	2.955	-0.127	0	3.603	1.664	0	2.846
N17	-1.391	0	3.979	2.713	0	2.216	0.777	0	4.636	1.841	0	4.207
C18	-1.513	0	5.337	3.797	0	3.042	0.117	0	5.83	3.174	0	4.502
C19	-0.24	0	5.877	3.337	0	4.346	-1.24	0	5.569	3.875	0	3.312
C20	0.679	0	4.794	1.918	0	4.294	-1.396	0	4.158	2.92	0	2.26
I21	3.454	0	2.271	-1.811	0	4.641	3.402	0	2.229	-1.672	0	4.609
H22	3.008	0	-4.425	1.59	0	-4.076	2.915	0	-4.466	1.519	0	-4.194
H23	-1.139	0	-5.649	-2.63	0	-5.025	-1.24	0	-5.663	-2.725	0	-5.029
H24	2.362	0	-2.047	1.095	0	-1.651	2.285	0	-2.084	1.089	0	-1.757

H25	-2.857	0	-3.44	-4.199	0	-2.7	-2.943	0	-3.442	-4.231	0	-2.665
H26	-2.727	0	-0.944	-3.903	0	-0.225	-2.797	0	-0.948	-3.87	0	-0.198
H27	-2.159	0	3.318	2.742	0	1.204	1.784	0	4.533	1.097	0	4.894
H28	-2.485	0	5.807	4.801	0	2.642	0.663	0	6.763	3.512	0	5.528
H29	0.001	0	6.931	3.953	0	5.235	-2.027	0	6.31	4.951	-0.001	3.211
H30	1.757	0	4.853	1.234	0	5.13	-2.322	0	3.598	3.112	0	1.196

Breitfussin A analog isomer 5												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	2.16	0.14	3.919	1.255	-1.183	3.711	2.39	0.098	3.823	1.091	-1.108	3.752
C2	1.314	0.244	5.039	0.364	-1.134	4.8	1.591	0.128	4.98	0.19	-0.946	4.822
C3	-0.062	0.294	4.935	-0.969	-0.797	4.67	0.21	0.12	4.939	-1.118	-0.536	4.652
C4	-0.584	0.236	3.639	-1.4	-0.487	3.375	-0.365	0.081	3.664	-1.512	-0.272	3.335
C5	0.226	0.133	2.483	-0.532	-0.492	2.259	0.397	0.05	2.472	-0.631	-0.394	2.235
C6	1.622	0.084	2.643	0.81	-0.865	2.438	1.799	0.059	2.57	0.682	-0.84	2.456
N7	-1.895	0.265	3.23	-2.657	-0.16	2.924	-1.694	0.069	3.312	-2.742	0.101	2.845
C8	-1.959	0.187	1.875	-2.626	0.033	1.576	-1.814	0.034	1.96	-2.682	0.211	1.489
C9	-0.68	0.103	1.355	-1.34	-0.15	1.116	-0.556	0.02	1.384	-1.403	-0.075	1.062
C10	-0.31	0.006	-0.036	-0.91	-0.048	-0.265	-0.242	-0.024	-0.024	-0.947	-0.069	-0.315
Br11	2.11	0.322	6.781	1.035	-1.573	6.542	2.461	0.184	6.687	0.81	-1.331	6.596
C12	-0.977	-0.035	-1.231	0.138	0.569	-0.886	-0.958	-0.014	-1.192	0.133	0.474	-0.948
C13	0.047	-0.133	-2.219	-0.028	0.262	-2.271	0.024	-0.079	-2.227	-0.021	0.101	-2.32
N14	1.231	-0.15	-1.647	-1.103	-0.477	-2.443	1.23	-0.124	-1.704	-1.121	-0.604	-2.471
O15	1.01	-0.062	-0.288	-1.652	-0.675	-1.194	1.063	-0.091	-0.334	-1.694	-0.717	-1.223
C16	-0.036	-0.212	-3.669	0.768	0.643	-3.425	-0.106	-0.099	-3.678	0.803	0.382	-3.487
N17	1.114	-0.267	-4.418	0.357	0.304	-4.691	-1.304	-0.025	-4.342	1.927	1.168	-3.453
C18	0.805	-0.344	-5.741	1.262	0.743	-5.607	-1.094	-0.064	-5.686	2.472	1.252	-4.697
C19	-0.572	-0.34	-5.859	2.284	1.379	-4.928	0.268	-0.166	-5.904	1.688	0.507	-5.56
C20	-1.107	-0.256	-4.548	1.973	1.319	-3.545	0.895	-0.188	-4.635	0.631	-0.044	-4.796
I21	-3.003	0.037	-1.513	1.515	1.793	0.007	-2.996	0.087	-1.378	1.545	1.679	-0.082
H22	3.235	0.104	4.055	2.289	-1.47	3.869	3.47	0.106	3.911	2.103	-1.449	3.943
H23	-0.711	0.375	5.801	-1.652	-0.779	5.513	-0.403	0.144	5.833	-1.81	-0.434	5.481
H24	2.283	0.004	1.787	1.493	-0.911	1.596	2.424	0.036	1.684	1.37	-0.978	1.628

H25	-2.699	0.337	3.842	-3.484	-0.073	3.503	-2.472	0.086	3.96	-3.569	0.27	3.404
H26	-2.914	0.197	1.372	-3.522	0.304	1.033	-2.79	0.017	1.5	-3.552	0.502	0.915
H27	2.053	-0.251	-4.038	-0.496	-0.198	-4.906	-2.213	0.05	-3.902	2.296	1.624	-2.628
H28	1.582	-0.395	-6.49	1.109	0.572	-6.663	-1.924	-0.017	-6.376	3.368	1.831	-4.87
H29	-1.131	-0.39	-6.783	3.155	1.838	-5.375	0.754	-0.219	-6.869	1.861	0.375	-6.619
H30	-2.15	-0.232	-4.275	2.561	1.714	-2.731	1.954	-0.26	-4.427	-0.169	-0.682	-5.147

Breitfussin A analog isomer 6												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	-4.368	0.648	1.017	-3.988	-0.723	-0.19	-4.362	0.704	1.146	-3.794	-1.326	0.296
C2	-5.166	0.921	-0.109	-4.714	-0.358	-1.341	-5.166	1.017	0.035	-4.678	-1.175	-0.791
C3	-4.655	0.99	-1.391	-4.117	0.115	-2.493	-4.668	1.103	-1.251	-4.275	-0.739	-2.039
C4	-3.279	0.769	-1.517	-2.721	0.227	-2.46	-3.299	0.858	-1.398	-2.914	-0.438	-2.175
C5	-2.437	0.489	-0.415	-1.957	-0.106	-1.317	-2.45	0.538	-0.311	-1.998	-0.552	-1.102
C6	-3.007	0.432	0.869	-2.609	-0.603	-0.177	-3.006	0.465	0.978	-2.454	-1.016	0.143
N7	-2.5	0.772	-2.648	-1.847	0.621	-3.444	-2.532	0.87	-2.537	-2.211	-0.023	-3.279
C8	-1.206	0.507	-2.315	-0.565	0.543	-2.976	-1.24	0.574	-2.224	-0.892	0.122	-2.955
C9	-1.103	0.324	-0.951	-0.578	0.105	-1.673	-1.125	0.36	-0.865	-0.708	-0.187	-1.627
C10	0.093	0.007	-0.184	0.592	-0.121	-0.828	0.072	0.001	-0.12	0.561	-0.165	-0.905
Br11	-7.044	1.204	0.151	-6.623	-0.544	-1.306	-7.035	1.335	0.325	-6.528	-1.609	-0.523
C12	1.458	-0.142	-0.59	0.86	0.4	0.472	1.429	-0.167	-0.545	0.881	0.517	0.307
C13	2.134	-0.449	0.557	2.088	-0.102	0.801	2.112	-0.512	0.587	2.197	0.224	0.534
O14	1.258	-0.482	1.575	2.52	-0.868	-0.217	1.249	-0.551	1.613	2.631	-0.576	-0.456
N15	-0.014	-0.199	1.112	1.579	-0.884	-1.233	-0.021	-0.232	1.172	1.604	-0.823	-1.35
C16	3.508	-0.731	0.896	2.971	0.021	1.933	3.482	-0.83	0.912	3.169	0.579	1.537
N17	3.857	-1.028	2.192	4.195	-0.605	1.945	4.5	-0.851	-0.009	2.891	1.416	2.59
C18	5.195	-1.255	2.269	4.832	-0.345	3.118	5.665	-1.188	0.603	4	1.564	3.361
C19	5.731	-1.104	1.002	4.011	0.464	3.885	5.405	-1.392	1.948	5.02	0.812	2.804
C20	4.666	-0.772	0.13	2.833	0.698	3.138	4.023	-1.166	2.146	4.496	0.187	1.647
I21	2.271	0.055	-2.457	-0.294	1.728	1.512	2.226	0.06	-2.419	-0.343	1.774	1.357
H22	-4.819	0.607	2.002	-4.512	-1.099	0.682	-4.802	0.65	2.135	-4.166	-1.684	1.25
H23	-5.274	1.201	-2.256	-4.685	0.38	-3.379	-5.293	1.345	-2.104	-4.963	-0.641	-2.872
H24	-2.396	0.221	1.74	-2.043	-0.893	0.703	-2.39	0.223	1.836	-1.765	-1.14	0.973

H25	-2.831	0.94	-3.59	-2.107	0.928	-4.373	-2.87	1.064	-3.471	-2.607	0.152	-4.195
H26	-0.448	0.464	-3.081	0.274	0.819	-3.6	-0.492	0.532	-3	-0.17	0.45	-3.69
H27	3.217	-1.076	2.975	4.573	-1.173	1.197	4.399	-0.646	-0.996	1.996	1.859	2.763
H28	5.659	-1.506	3.211	5.814	-0.751	3.315	6.584	-1.257	0.04	3.98	2.19	4.242
H29	6.772	-1.219	0.736	4.237	0.842	4.871	6.131	-1.671	2.699	6.026	0.725	3.188
H30	4.73	-0.584	-0.931	1.978	1.287	3.436	3.473	-1.236	3.075	5.015	-0.475	0.967

Breitfussin A analog isomer 7												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	-0.272	0.212	-4.374	-1.633	-0.804	-2.143	-0.191	0.294	-4.425	-1.72	-0.572	-2.157
C2	-1.574	0.745	-4.376	-2.965	-0.353	-2.077	-1.505	0.794	-4.479	-2.999	0.013	-2.092
C3	-2.269	1.033	-3.218	-3.521	0.181	-0.931	-2.27	1.016	-3.35	-3.512	0.57	-0.937
C4	-1.601	0.766	-2.019	-2.677	0.258	0.183	-1.66	0.717	-2.127	-2.677	0.536	0.185
C5	-0.293	0.229	-1.967	-1.327	-0.169	0.16	-0.341	0.215	-2.023	-1.376	-0.022	0.162
C6	0.373	-0.046	-3.174	-0.814	-0.717	-1.029	0.395	0.005	-3.203	-0.908	-0.594	-1.034
N7	-2.032	0.946	-0.725	-2.955	0.714	1.449	-2.164	0.835	-0.854	-2.92	0.986	1.462
C8	-1.064	0.551	0.143	-1.849	0.595	2.232	-1.234	0.434	0.051	-1.838	0.74	2.248
C9	0.033	0.096	-0.567	-0.813	0.062	1.491	-0.086	0.041	-0.611	-0.853	0.127	1.5
C10	1.267	-0.379	0.007	0.51	-0.2	2.016	1.137	-0.42	0	0.437	-0.276	2.014
Br11	-2.418	1.08	-6.065	-4.054	-0.497	-3.648	-2.261	1.184	-6.197	-4.074	0.027	-3.68
C12	1.687	-0.591	1.298	1.766	-0.244	1.464	1.548	-0.637	1.295	1.685	-0.396	1.457
C13	3.025	-1.028	1.113	2.582	-0.545	2.59	2.896	-1.052	1.118	2.47	-0.836	2.559
N14	3.386	-1.082	-0.139	1.907	-0.667	3.698	3.27	-1.094	-0.129	1.788	-0.964	3.661
O15	2.266	-0.675	-0.845	0.592	-0.447	3.339	2.152	-0.7	-0.842	0.495	-0.609	3.32
I16	4.354	-1.552	2.592	4.628	-0.762	2.625	4.214	-1.568	2.612	4.489	-1.228	2.527
C17	0.94	-0.434	2.542	2.171	0.028	0.091	0.821	-0.505	2.553	2.123	-0.066	0.106
N18	-0.156	-1.211	2.823	1.725	1.137	-0.58	1.275	0.316	3.555	2.688	-1.004	-0.72
C19	-0.698	-0.842	4.02	2.183	1.123	-1.865	0.454	0.231	4.641	2.958	-0.452	-1.938
C20	0.064	0.192	4.529	2.949	-0.015	-2.03	-0.555	-0.663	4.34	2.561	0.87	-1.903
C21	1.103	0.451	3.592	2.943	-0.71	-0.789	-0.32	-1.134	3.019	2.033	1.116	-0.605
H22	0.23	0.004	-5.313	-1.248	-1.222	-3.066	0.365	0.136	-5.342	-1.37	-1.008	-3.086
H23	-3.274	1.443	-3.225	-4.551	0.517	-0.884	-3.283	1.401	-3.396	-4.503	1.008	-0.89
H24	1.377	-0.455	-3.181	0.21	-1.075	-1.087	1.409	-0.378	-3.172	0.073	-1.055	-1.092

H25	-2.933	1.321	-0.455	-3.844	1.089	1.756	-3.093	1.166	-0.62	-3.77	1.441	1.772
H26	-1.221	0.624	1.211	-1.865	0.909	3.266	-1.45	0.453	1.11	-1.831	1.031	3.289
H27	-0.504	-1.954	2.229	1.135	1.856	-0.179	2.096	0.905	3.487	2.861	-1.969	-0.465
H28	-1.569	-1.345	4.414	1.938	1.922	-2.55	0.651	0.81	5.532	3.415	-1.037	-2.724
H29	-0.105	0.701	5.468	3.456	-0.311	-2.937	-1.364	-0.95	4.997	2.647	1.579	-2.715
H30	1.881	1.2	3.661	3.42	-1.653	-0.562	-0.906	-1.855	2.463	1.626	2.043	-0.224

Breitfussin A analog isomer 8												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	-1.553	2.242	-1.485	-1.322	2.282	-1.28	-1.218	1.524	2.022	-1.031	1.602	1.877
C2	-2.912	2.1	-1.143	-2.703	2.164	-1.025	-2.62	1.514	1.876	-2.436	1.622	1.774
C3	-3.445	0.934	-0.628	-3.301	0.984	-0.628	-3.286	0.647	1.032	-3.15	0.737	0.99
C4	-2.548	-0.128	-0.454	-2.45	-0.119	-0.484	-2.484	-0.242	0.304	-2.393	-0.205	0.281
C5	-1.175	-0.026	-0.781	-1.058	-0.045	-0.73	-1.074	-0.263	0.418	-0.981	-0.261	0.357
C6	-0.682	1.179	-1.304	-0.497	1.179	-1.132	-0.443	0.636	1.294	-0.301	0.66	1.17
N7	-2.764	-1.391	0.038	-2.735	-1.406	-0.102	-2.84	-1.201	-0.611	-2.803	-1.195	-0.577
C8	-1.585	-2.087	0.042	-1.584	-2.145	-0.088	-1.714	-1.821	-1.083	-1.71	-1.87	-1.051
C9	-0.577	-1.293	-0.45	-0.522	-1.356	-0.468	-0.601	-1.28	-0.484	-0.565	-1.337	-0.506
C10	0.82	-1.678	-0.635	0.869	-1.778	-0.608	0.786	-1.684	-0.698	0.803	-1.792	-0.738
Br11	-4.074	3.605	-1.401	-3.801	3.722	-1.239	-3.645	2.769	2.903	-3.398	2.947	2.774
C12	2.014	-1.146	-0.035	2.054	-1.223	-0.011	1.901	-0.927	-1.2	1.95	-1.036	-1.168
N13	3.091	-1.753	-0.484	3.137	-1.856	-0.404	3.002	-1.645	-1.221	3.029	-1.784	-1.231
O14	2.651	-2.702	-1.392	2.71	-2.837	-1.284	2.659	-2.896	-0.736	2.641	-3.051	-0.83
C15	1.321	-2.631	-1.463	1.382	-2.765	-1.388	1.359	-2.887	-0.434	1.338	-3.026	-0.543
I16	0.381	-3.898	-2.765	0.475	-4.075	-2.673	0.576	-4.605	0.351	0.51	-4.763	0.149
C17	2.131	-0.092	0.957	2.156	-0.102	0.911	1.921	0.45	-1.664	2.021	0.381	-1.489
N18	3.36	0.382	1.343	1.11	0.291	1.706	3.104	1.075	-1.971	0.937	1.081	-1.955
C19	3.208	1.341	2.298	1.479	1.361	2.462	2.859	2.341	-2.408	1.278	2.385	-2.15
C20	1.856	1.492	2.542	2.79	1.674	2.15	1.492	2.544	-2.39	2.608	2.537	-1.8
C21	1.17	0.585	1.693	3.221	0.747	1.167	0.895	1.347	-1.918	3.08	1.267	-1.381
H22	-1.191	3.182	-1.887	-0.908	3.235	-1.589	-0.75	2.227	2.702	-0.524	2.323	2.509
H23	-4.494	0.838	-0.369	-4.365	0.907	-0.434	-4.366	0.648	0.929	-4.232	0.763	0.919
H24	0.369	1.285	-1.561	0.57	1.266	-1.323	0.638	0.642	1.399	0.783	0.643	1.243

H25	-3.654	-1.754	0.358	-3.654	-1.758	0.139	-3.786	-1.414	-0.901	-3.763	-1.392	-0.831
H26	-1.544	-3.107	0.399	-1.597	-3.188	0.198	-1.782	-2.608	-1.822	-1.823	-2.685	-1.753
H27	4.246	0.068	0.967	0.202	-0.157	1.743	4.022	0.657	-1.878	0.024	0.685	-2.146
H28	4.067	1.839	2.724	0.786	1.813	3.157	3.671	2.995	-2.691	0.555	3.096	-2.521
H29	1.411	2.178	3.249	3.367	2.483	2.576	0.981	3.451	-2.681	3.17	3.46	-1.835
H30	0.102	0.436	1.627	4.187	0.703	0.682	-0.161	1.155	-1.783	4.069	1.018	-1.02

Breitfussin A analog isomer 9												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	-4.352	-0.325	0.462	-2.136	-1.815	-0.18	-4.431	-0.236	-0.065	-2.114	-1.84	-0.222
C2	-4.297	-1.535	1.178	-1.976	-3.013	0.541	-4.497	-1.64	0.014	-1.968	-3.04	0.499
C3	-3.11	-2.16	1.506	-0.766	-3.412	1.073	-3.374	-2.441	0.094	-0.768	-3.443	1.051
C4	-1.941	-1.516	1.086	0.313	-2.546	0.862	-2.144	-1.775	0.092	0.316	-2.578	0.861
C5	-1.948	-0.299	0.364	0.199	-1.324	0.155	-2.028	-0.366	0.017	0.214	-1.354	0.157
C6	-3.182	0.296	0.054	-1.054	-0.972	-0.378	-3.201	0.404	-0.063	-1.028	-0.998	-0.398
N7	-0.63	-1.89	1.265	1.625	-2.69	1.247	-0.874	-2.297	0.158	1.622	-2.724	1.266
C8	0.194	-0.973	0.693	2.348	-1.623	0.817	0.04	-1.293	0.125	2.352	-1.654	0.851
C9	-0.563	0.032	0.119	1.523	-0.744	0.143	-0.612	-0.078	0.04	1.537	-0.774	0.168
C10	-0.045	1.195	-0.555	1.976	0.496	-0.447	0.013	1.222	0.007	1.98	0.469	-0.423
Br11	-5.947	-2.345	1.723	-3.506	-4.144	0.777	-6.224	-2.472	0.011	-3.504	-4.169	0.706
C12	1.224	1.604	-0.891	1.375	1.695	-0.747	1.315	1.663	-0.034	1.37	1.67	-0.678
C13	0.983	2.862	-1.504	2.455	2.449	-1.288	1.155	3.076	-0.016	2.416	2.422	-1.281
N14	-0.278	3.19	-1.542	3.579	1.792	-1.316	-0.089	3.46	0.028	3.536	1.765	-1.376
O15	-0.935	2.126	-0.945	3.281	0.553	-0.783	-0.817	2.284	0.035	3.265	0.523	-0.831
I16	2.398	4.129	-2.294	2.4	4.393	-1.958	2.669	4.467	-0.07	2.285	4.364	-1.95
C17	2.494	0.914	-0.69	0.002	2.12	-0.506	2.565	0.913	-0.105	0.02	2.103	-0.338
N18	2.768	-0.283	-1.304	-0.587	1.975	0.724	3.542	1.065	0.847	-0.87	2.511	-1.299
C19	3.999	-0.732	-0.925	-1.89	2.375	0.669	4.623	0.294	0.536	-2.073	2.806	-0.726
C20	4.539	0.193	-0.053	-2.15	2.796	-0.621	4.344	-0.373	-0.64	-1.961	2.586	0.634
C21	3.584	1.238	0.097	-0.95	2.635	-1.367	3.041	0.023	-1.05	-0.633	2.142	0.88
H22	-5.312	0.123	0.23	-3.107	-1.551	-0.583	-5.343	0.346	-0.127	-3.078	-1.575	-0.643
H23	-3.073	-3.093	2.058	-0.644	-4.341	1.618	-3.431	-3.522	0.155	-0.658	-4.374	1.595
H24	-3.234	1.229	-0.497	-1.188	-0.056	-0.945	-3.16	1.486	-0.123	-1.15	-0.08	-0.964

H25	-0.318	-2.721	1.753	2	-3.472	1.771	-0.647	-3.283	0.216	1.988	-3.505	1.797
H26	1.268	-1.096	0.738	3.406	-1.548	1.029	1.099	-1.509	0.166	3.407	-1.581	1.081
H27	2.146	-0.754	-1.95	-0.12	1.614	1.548	3.462	1.657	1.665	-0.663	2.569	-2.289
H28	4.393	-1.662	-1.31	-2.519	2.338	1.547	5.496	0.281	1.173	-2.903	3.155	-1.324
H29	5.508	0.126	0.421	-3.094	3.176	-0.984	5.004	-1.062	-1.15	-2.743	2.733	1.365
H30	3.667	2.124	0.712	-0.796	2.842	-2.418	2.504	-0.294	-1.934	-0.193	1.872	1.832

Breitfussin A analog isomer 10												
ATOM	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
C1	-2.401	-0.855	-1.624	-2.424	-0.959	-1.676	-3.834	-0.356	-0.227	-3.146	-0.38	3.377
C2	-2.529	-2.252	-1.5	-2.552	-2.354	-1.52	-3.963	-1.724	0.083	-3.379	-1.748	3.127
C3	-1.502	-3.071	-1.073	-1.532	-3.16	-1.052	-2.943	-2.477	0.632	-2.63	-2.493	2.236
C4	-0.295	-2.433	-0.759	-0.333	-2.51	-0.73	-1.742	-1.798	0.878	-1.604	-1.808	1.572
C5	-0.126	-1.032	-0.865	-0.164	-1.112	-0.868	-1.576	-0.422	0.595	-1.346	-0.433	1.785
C6	-1.2	-0.241	-1.307	-1.23	-0.336	-1.351	-2.639	0.298	0.027	-2.129	0.279	2.707
N7	0.889	-2.959	-0.307	0.844	-3.023	-0.244	-0.558	-2.258	1.397	-0.691	-2.262	0.654
C8	1.794	-1.952	-0.115	1.744	-2.008	-0.064	0.346	-1.231	1.454	0.132	-1.233	0.28
C9	1.222	-0.744	-0.445	1.174	-0.811	-0.431	-0.227	-0.081	0.965	-0.223	-0.088	0.952
C10	1.863	0.568	-0.416	1.818	0.499	-0.429	0.381	1.242	0.859	0.386	1.234	0.839
Br11	-4.218	-3.048	-1.943	-4.229	-3.166	-1.98	-5.642	-2.581	-0.28	-4.803	-2.61	4.079
C12	1.493	1.711	0.25	1.467	1.652	0.23	1.45	1.677	0.117	1.646	1.668	1.166
O13	2.335	2.715	-0.059	2.32	2.643	-0.094	1.654	2.991	0.337	1.764	2.982	0.888
N14	3.295	2.264	-0.947	3.272	2.172	-0.983	0.712	3.471	1.231	0.571	3.463	0.374
C15	3.001	1.01	-1.147	2.958	0.92	-1.169	-0.02	2.434	1.525	-0.219	2.427	0.353
C16	0.437	2.026	1.18	0.426	1.98	1.171	2.341	1.037	-0.819	2.806	1.028	1.735
N17	-0.402	1.071	1.7	0.271	3.258	1.651	3.358	1.733	-1.427	3.961	1.732	1.977
C18	-1.291	1.655	2.547	-0.765	3.296	2.531	4.032	0.913	-2.278	4.891	0.913	2.535
C19	-1.03	3.014	2.579	-1.294	2.021	2.628	3.444	-0.339	-2.226	4.335	-0.348	2.66
C20	0.065	3.252	1.714	-0.543	1.184	1.768	2.374	-0.264	-1.302	3.015	-0.279	2.154
I21	4.129	-0.116	-2.447	4.062	-0.234	-2.464	-1.567	2.614	2.87	-2.135	2.605	-0.374
H22	-3.242	-0.262	-1.966	-3.26	-0.378	-2.049	-4.669	0.181	-0.663	-3.763	0.151	4.093
H23	-1.614	-4.146	-0.981	-1.643	-4.232	-0.937	-3.055	-3.532	0.859	-2.816	-3.547	2.059
H24	-1.095	0.837	-1.396	-1.126	0.74	-1.466	-2.529	1.351	-0.215	-1.939	1.331	2.902

H25	1.066	-3.94	-0.131	1.02	-3.999	-0.043	-0.379	-3.208	1.699	-0.634	-3.209	0.3
H26	2.791	-2.164	0.247	2.736	-2.209	0.318	1.344	-1.393	1.839	0.921	-1.39	-0.444
H27	-0.36	0.078	1.501	0.84	4.055	1.391	3.578	2.709	-1.274	4.101	2.716	1.778
H28	-2.037	1.063	3.058	-1.044	4.219	3.016	4.872	1.28	-2.849	5.871	1.287	2.796
H29	-1.571	3.749	3.158	-2.129	1.727	3.249	3.753	-1.208	-2.788	4.827	-1.22	3.069
H30	0.535	4.201	1.496	-0.683	0.126	1.597	1.701	-1.06	-1.016	2.294	-1.083	2.097

Chemical Shielding Tensors of the ten isomeric breitfussin A structures

Isomer 1 (conformer 1)

1 C Isotropic = 57.6297 Anisotropy = 143.1677
XX= 24.2615 YX= 30.0016 ZX= -36.9352
XY= 31.1471 YY= 115.5978 ZY= 66.3168
XZ= -39.6819 YZ= 66.4719 ZZ= 33.0298
Eigenvalues: -40.2691 60.0834 153.0749
2 C Isotropic = 47.3278 Anisotropy = 112.8381
XX= -33.4794 YX= -0.9408 ZX= 26.3834
XY= -2.0373 YY= 108.5921 ZY= 26.8563
XZ= 29.7177 YZ= 26.8305 ZZ= 66.8708
Eigenvalues: -41.2555 60.6856 122.5532
3 C Isotropic = 69.9599 Anisotropy = 125.0036
XX= 53.5081 YX= -5.8632 ZX= 26.9646
XY= -7.6487 YY= 122.1061 ZY= 60.5439
XZ= 30.9435 YZ= 59.9934 ZZ= 34.2656
Eigenvalues: -9.6506 66.2347 153.2957
4 C Isotropic = 47.2033 Anisotropy = 140.2436
XX= 9.8559 YX= 21.6754 ZX= -20.8061
XY= 21.8474 YY= 106.1645 ZY= 62.4382
XZ= -20.8949 YZ= 62.0715 ZZ= 25.5895
Eigenvalues: -29.4959 30.4068 140.6990
5 C Isotropic = 59.8032 Anisotropy = 159.8967
XX= -3.6428 YX= 5.7106 ZX= 15.2909
XY= 3.8478 YY= 134.1240 ZY= 60.8245
XZ= 18.3385 YZ= 60.2538 ZZ= 48.9285
Eigenvalues: -10.2847 23.2934 166.4010
6 C Isotropic = 59.0738 Anisotropy = 168.7181
XX= 40.5502 YX= 2.2505 ZX= 16.2648
XY= 3.8553 YY= 127.2676 ZY= 83.6834
XZ= 11.5218 YZ= 84.2403 ZZ= 9.4035
Eigenvalues: -35.8136 41.4824 171.5525
7 N Isotropic = 115.0016 Anisotropy = 84.4562
XX= 129.7510 YX= 4.4094 ZX= -1.5685
XY= 2.4867 YY= 143.6894 ZY= 52.4246
XZ= 3.0380 YZ= 51.8680 ZZ= 71.5645
Eigenvalues: 44.2150 129.4841 171.3057
8 C Isotropic = 61.5802 Anisotropy = 116.0855
XX= -5.1205 YX= 10.7225 ZX= 1.9860
XY= 6.0928 YY= 120.2648 ZY= 34.7722
XZ= 12.4273 YZ= 35.2978 ZZ= 69.5963
Eigenvalues: -6.0406 51.8107 138.9705
9 C Isotropic = 75.8719 Anisotropy = 108.8794
XX= 20.8006 YX= -1.8326 ZX= 23.1290
XY= 2.8656 YY= 129.1339 ZY= 36.2087
XZ= 11.3213 YZ= 36.3886 ZZ= 77.6812
Eigenvalues: 15.0946 64.0628 148.4582
10 C Isotropic = 35.0502 Anisotropy = 86.8653
XX= 53.7484 YX= 1.0027 ZX= 0.6670
XY= 1.2193 YY= 66.5121 ZY= 53.8364
XZ= 1.2978 YZ= 52.9578 ZZ= -15.1098
Eigenvalues: -41.5075 53.6978 92.9604
11 Br Isotropic = 1895.0181 Anisotropy = 1568.9165

XX= 2870.8090 YX= 37.2039 ZX= -308.5910
XY= 43.2962 YY= 1343.2078 ZY= -50.4895
XZ= -326.0561 YZ= -52.0960 ZZ= 1471.0374
Eigenvalues: 1320.5035 1423.5884 2940.9624
12 C Isotropic = 65.5552 Anisotropy = 47.4632
XX= 73.2261 YX= 12.1302 ZX= -23.7891
XY= 20.6214 YY= 74.5841 ZY= 22.3421
XZ= -44.1676 YZ= 21.2224 ZZ= 48.8555
Eigenvalues: 12.9121 86.5562 97.1974
13 N Isotropic = -14.3168 Anisotropy = 295.8329
XX= -54.8701 YX= 7.1217 ZX= 8.3732
XY= 16.7640 YY= 113.8848 ZY= 139.2197
XZ= -10.2437 YZ= 140.0924 ZZ= -101.9651
Eigenvalues: -170.8603 -54.9952 182.9051
14 C Isotropic = 29.1243 Anisotropy = 77.5056
XX= 26.7067 YX= -11.2528 ZX= 28.3270
XY= -16.4586 YY= 62.8356 ZY= 38.1658
XZ= 36.0319 YZ= 38.9713 ZZ= -2.1693
Eigenvalues: -38.8232 45.4015 80.7947
15 O Isotropic = 30.1059 Anisotropy = 225.5712
XX= -6.0237 YX= 24.2572 ZX= -30.8654
XY= -3.0774 YY= 128.4986 ZY= 105.5995
XZ= 20.1495 YZ= 103.9988 ZZ= -32.1570
Eigenvalues: -85.0156 -5.1533 180.4867
16 C Isotropic = 62.4244 Anisotropy = 99.1783
XX= 45.6056 YX= -8.8706 ZX= 24.5875
XY= -4.6073 YY= 107.2453 ZY= 44.1303
XZ= 16.7465 YZ= 45.1629 ZZ= 34.4223
Eigenvalues: 2.4387 56.2912 128.5433
17 N Isotropic = 97.3374 Anisotropy = 125.2887
XX= 10.5826 YX= 10.6410 ZX= -8.1863
XY= 9.3839 YY= 165.0198 ZY= 31.7114
XZ= -4.1520 YZ= 31.6179 ZZ= 116.4098
Eigenvalues: 9.2705 101.8785 180.8632
18 C Isotropic = 62.7973 Anisotropy = 118.2914
XX= 57.3899 YX= -1.8126 ZX= 10.6275
XY= -4.8117 YY= 112.8125 ZY= 59.6475
XZ= 17.0520 YZ= 59.4269 ZZ= 18.1896
Eigenvalues: -13.2830 60.0167 141.6583
19 C Isotropic = 71.5040 Anisotropy = 134.3161
XX= 40.2979 YX= 16.2061 ZX= -24.0438
XY= 16.9231 YY= 132.0682 ZY= 57.9695
XZ= -24.5470 YZ= 59.0597 ZZ= 42.1459
Eigenvalues: -5.3130 58.7769 161.0481
20 C Isotropic = 72.0526 Anisotropy = 138.9886
XX= 7.8139 YX= -2.8192 ZX= 18.9209
XY= -5.2526 YY= 142.1571 ZY= 46.8812
XZ= 22.2076 YZ= 46.9442 ZZ= 66.1868
Eigenvalues: -1.4528 52.8989 164.7117
21 I Isotropic = 3746.2597 Anisotropy = 1835.2138
XX= 4002.7682 YX= -466.4545 ZX= 878.2975
XY= -427.4958 YY= 3509.3589 ZY= -225.2620
XZ= 970.0781 YZ= -263.5911 ZZ= 3726.6520
Eigenvalues: 2906.1890 3362.8546 4969.7356
22 H Isotropic = 24.0893 Anisotropy = 10.4017

XX= 27.3564 YX= 1.2224 ZX= -3.8020
XY= 1.0545 YY= 19.5845 ZY= -3.5454
XZ= -3.5492 YZ= -3.6204 ZZ= 25.3269
Eigenvalues: 17.8243 23.4199 31.0238
23 H Isotropic = 24.1793 Anisotropy = 10.3747
XX= 30.0816 YX= -2.0844 ZX= 2.0485
XY= -1.7209 YY= 19.3544 ZY= -3.1205
XZ= 1.4678 YZ= -2.9978 ZZ= 23.1020
Eigenvalues: 17.5858 23.8564 31.0958
24 H Isotropic = 23.0377 Anisotropy = 10.7044
XX= 30.0716 YX= -0.9843 ZX= -0.4481
XY= -0.7255 YY= 16.9646 ZY= -3.4317
XZ= -1.1604 YZ= -3.4242 ZZ= 22.0768
Eigenvalues: 15.1598 23.7793 30.1740
25 H Isotropic = 24.0199 Anisotropy = 9.2688
XX= 26.5126 YX= -0.5629 ZX= -0.5995
XY= -0.1087 YY= 18.5250 ZY= -5.9205
XZ= -1.1646 YZ= -5.9934 ZZ= 27.0221
Eigenvalues: 15.4122 26.4484 30.1991
26 H Isotropic = 23.3317 Anisotropy = 13.9753
XX= 28.9944 YX= 2.2014 ZX= -5.7234
XY= 0.8039 YY= 16.9541 ZY= -4.7234
XZ= -3.3455 YZ= -4.9423 ZZ= 24.0467
Eigenvalues: 14.4664 22.8802 32.6486
27 H Isotropic = 22.8817 Anisotropy = 7.6226
XX= 27.1825 YX= -0.9159 ZX= 0.8031
XY= -0.9078 YY= 17.3575 ZY= -4.4456
XZ= 0.8110 YZ= -4.4129 ZZ= 24.1051
Eigenvalues: 15.1458 25.5359 27.9634
28 H Isotropic = 24.6761 Anisotropy = 3.4698
XX= 25.8951 YX= 0.1805 ZX= -0.7654
XY= -0.3712 YY= 22.3019 ZY= -2.2940
XZ= 0.2731 YZ= -2.2916 ZZ= 25.8314
Eigenvalues: 21.1653 25.8737 26.9893
29 H Isotropic = 25.1323 Anisotropy = 2.7885
XX= 26.1870 YX= 0.0037 ZX= -0.3881
XY= -0.2886 YY= 23.1278 ZY= -1.8319
XZ= 0.0497 YZ= -1.8904 ZZ= 26.0821
Eigenvalues: 22.2186 26.1870 26.9913
30 H Isotropic = 24.4593 Anisotropy = 5.8976
XX= 25.2855 YX= -0.6184 ZX= 0.6072
XY= -0.4403 YY= 21.4508 ZY= -3.2856
XZ= 0.2964 YZ= -3.3527 ZZ= 26.6414
Eigenvalues: 19.8185 25.1683 28.3910

Isomer 1 (conformer 2)

1 C Isotropic = 58.3519 Anisotropy = 143.9843
XX= -3.1689 YX= -28.3088 ZX= -42.5953
XY= -30.4572 YY= 148.8593 ZY= -8.4192
XZ= -46.6294 YZ= -7.5996 ZZ= 29.3652
Eigenvalues: -38.7915 59.5057 154.3415
2 C Isotropic = 47.1007 Anisotropy = 112.4769
XX= -3.7648 YX= -22.6456 ZX= 44.6223
XY= -25.5672 YY= 117.4567 ZY= 10.1025
XZ= 48.4381 YZ= 9.5752 ZZ= 27.6103
Eigenvalues: -41.2299 60.4467 122.0853
3 C Isotropic = 70.1023 Anisotropy = 124.7718
XX= 67.7794 YX= -14.6686 ZX= 2.7845
XY= -14.3982 YY= 150.6631 ZY= 6.6255
XZ= 8.9178 YZ= 5.1955 ZZ= -8.1356
Eigenvalues: -8.8963 65.9197 153.2835
4 C Isotropic = 47.5217 Anisotropy = 141.8241
XX= -8.5190 YX= -22.9918 ZX= -27.9746
XY= -25.7626 YY= 137.9530 ZY= 0.2100
XZ= -29.4960 YZ= -0.2971 ZZ= 13.1311
Eigenvalues: -30.8306 31.3246 142.0711
5 C Isotropic = 58.0574 Anisotropy = 165.2544
XX= 6.5997 YX= -27.6404 ZX= 11.8851
XY= -27.0851 YY= 163.5940 ZY= 0.7989
XZ= 14.6181 YZ= 3.0496 ZZ= 3.9784
Eigenvalues: -10.4520 16.3971 168.2270
6 C Isotropic = 58.8575 Anisotropy = 174.5604
XX= 38.2421 YX= -23.8097 ZX= -14.4321
XY= -17.9285 YY= 172.0351 ZY= -3.9896
XZ= -16.7642 YZ= -4.4882 ZZ= -33.7048
Eigenvalues: -37.2852 38.6266 175.2311
7 N Isotropic = 114.4477 Anisotropy = 88.6505
XX= 115.7211 YX= -9.1063 ZX= -32.6237
XY= -13.2987 YY= 171.2541 ZY= -3.1660
XZ= -24.3609 YZ= -0.7312 ZZ= 56.3677
Eigenvalues: 44.6184 125.1766 173.5480
8 C Isotropic = 60.4681 Anisotropy = 116.5474
XX= -2.4532 YX= -23.1558 ZX= 19.3442
XY= -22.2683 YY= 134.4903 ZY= 2.6161
XZ= 30.7164 YZ= 7.0874 ZZ= 49.3671
Eigenvalues: -16.0497 59.2876 138.1663
9 C Isotropic = 76.4209 Anisotropy = 106.8600
XX= 40.1195 YX= -15.9421 ZX= 34.2301
XY= -12.1920 YY= 145.8174 ZY= 4.2296
XZ= 27.8263 YZ= 5.0226 ZZ= 43.3257
Eigenvalues: 9.3340 72.2677 147.6609
10 C Isotropic = 36.9120 Anisotropy = 87.0878
XX= 28.6142 YX= 41.6429 ZX= 50.2024
XY= 36.6554 YY= 68.3264 ZY= -21.5553
XZ= 52.8929 YZ= -15.1127 ZZ= 13.7954
Eigenvalues: -44.9651 60.7307 94.9705
11 Br Isotropic = 1894.4484 Anisotropy = 1581.9162
XX= 2499.7647 YX= 217.8704 ZX= -662.8583
XY= 198.3528 YY= 1353.8494 ZY= -98.2061

XZ= -677.7279 YZ= -126.6668 ZZ= 1829.7310
Eigenvalues: 1317.0033 1417.2827 2949.0592
12 C Isotropic = 57.1534 Anisotropy = 48.9703
XX= 34.7021 YX= 48.4708 ZX= 4.8810
XY= 38.9951 YY= 49.4664 ZY= -1.8503
XZ= 17.5190 YZ= -18.2134 ZZ= 87.2916
Eigenvalues: -4.7224 86.3823 89.8002
13 N Isotropic = -15.6088 Anisotropy = 294.7350
XX= -19.3039 YX= 142.7644 ZX= 81.6914
XY= 137.2360 YY= 50.7746 ZY= 33.5743
XZ= 95.8664 YZ= 10.5006 ZZ= -78.2971
Eigenvalues: -170.3010 -57.4066 180.8812
14 C Isotropic = 26.7515 Anisotropy = 85.1500
XX= 47.3935 YX= 14.8796 ZX= 43.1028
XY= 30.7183 YY= 56.0857 ZY= 0.8456
XZ= 36.1533 YZ= 6.5901 ZZ= -23.2247
Eigenvalues: -41.3718 38.1081 83.5182
15 O Isotropic = 16.6641 Anisotropy = 221.1635
XX= 20.0812 YX= 93.5929 ZX= 72.9058
XY= 128.5627 YY= 54.5171 ZY= -2.6108
XZ= 40.8565 YZ= 40.9993 ZZ= -24.6059
Eigenvalues: -91.8651 -22.2490 164.1065
16 C Isotropic = 62.2790 Anisotropy = 100.1809
XX= 74.6670 YX= 36.0067 ZX= 30.9599
XY= 33.5216 YY= 93.4466 ZY= 15.5156
XZ= 37.1096 YZ= 10.0803 ZZ= 18.7235
Eigenvalues: 2.4983 55.2725 129.0663
17 N Isotropic = 96.9064 Anisotropy = 126.1366
XX= 114.7341 YX= 62.9507 ZX= -11.8841
XY= 62.1751 YY= 106.3296 ZY= 51.8777
XZ= -14.5139 YZ= 55.4060 ZZ= 69.6554
Eigenvalues: 7.5648 102.1568 180.9975
18 C Isotropic = 62.8163 Anisotropy = 118.9230
XX= 66.8540 YX= 46.7676 ZX= 50.2854
XY= 48.0706 YY= 98.9748 ZY= 2.1559
XZ= 45.5246 YZ= 6.1108 ZZ= 22.6202
Eigenvalues: -13.1021 59.4527 142.0984
19 C Isotropic = 71.6177 Anisotropy = 134.7840
XX= 62.5549 YX= 76.8097 ZX= 26.4170
XY= 76.9796 YY= 87.9722 ZY= 15.1623
XZ= 26.6293 YZ= 13.9144 ZZ= 64.3259
Eigenvalues: -4.5103 57.8896 161.4737
20 C Isotropic = 71.8929 Anisotropy = 140.9277
XX= 99.0001 YX= 51.4872 ZX= 18.8796
XY= 55.0488 YY= 101.3857 ZY= 41.4406
XZ= 16.3076 YZ= 43.8633 ZZ= 15.2927
Eigenvalues: -2.4709 52.3048 165.8447
21 I Isotropic = 3790.3919 Anisotropy = 1994.7777
XX= 4145.2838 YX= -931.3396 ZX= 213.3184
XY= -931.2846 YY= 4222.1467 ZY= -15.3208
XZ= 129.6763 YZ= 76.9594 ZZ= 3003.7452
Eigenvalues: 2933.3440 3317.5881 5120.2437
22 H Isotropic = 24.1873 Anisotropy = 10.4687
XX= 24.7724 YX= 1.5572 ZX= -3.6025
XY= 2.0644 YY= 18.6812 ZY= -1.2333

XZ= -2.9559 YZ= -1.1545 ZZ= 29.1085
Eigenvalues: 18.1749 23.2207 31.1665
23 H Isotropic = 24.0917 Anisotropy = 9.8035
XX= 30.2744 YX= 2.0428 ZX= 0.5327
XY= 2.1493 YY= 17.9919 ZY= -0.4508
XZ= -0.0195 YZ= -0.3897 ZZ= 24.0088
Eigenvalues: 17.6115 24.0363 30.6274
24 H Isotropic = 23.6397 Anisotropy = 11.1375
XX= 27.4731 YX= 3.5868 ZX= -2.5677
XY= 5.0427 YY= 20.9826 ZY= -3.4128
XZ= -2.0131 YZ= -2.9125 ZZ= 22.4634
Eigenvalues: 17.9055 21.9489 31.0647
25 H Isotropic = 23.7989 Anisotropy = 10.0133
XX= 25.5690 YX= 1.1400 ZX= 1.7770
XY= 1.0273 YY= 15.7443 ZY= -0.8569
XZ= 0.9474 YZ= -0.6053 ZZ= 30.0834
Eigenvalues: 15.5729 25.3493 30.4744
26 H Isotropic = 24.1939 Anisotropy = 6.1814
XX= 25.2474 YX= 0.0586 ZX= 0.3084
XY= 0.5593 YY= 19.3020 ZY= 0.7812
XZ= 1.5137 YZ= -0.3083 ZZ= 28.0322
Eigenvalues: 19.2819 24.9850 28.3148
27 H Isotropic = 22.8846 Anisotropy = 7.5040
XX= 22.8280 YX= -5.7405 ZX= -1.5105
XY= -5.8133 YY= 21.1717 ZY= -2.4080
XZ= -1.5103 YZ= -2.1934 ZZ= 24.6541
Eigenvalues: 15.3622 25.4043 27.8873
28 H Isotropic = 24.7235 Anisotropy = 3.4463
XX= 24.5811 YX= -2.3968 ZX= -0.8788
XY= -2.1664 YY= 23.5399 ZY= -1.0073
XZ= -1.7425 YZ= -0.2433 ZZ= 26.0496
Eigenvalues: 21.3509 25.7986 27.0210
29 H Isotropic = 25.2414 Anisotropy = 2.7464
XX= 25.2402 YX= -1.9651 ZX= -0.8187
XY= -1.9865 YY= 24.3095 ZY= -0.6386
XZ= -1.0812 YZ= -0.3979 ZZ= 26.1747
Eigenvalues: 22.4739 26.1781 27.0724
30 H Isotropic = 24.6143 Anisotropy = 5.8392
XX= 25.3623 YX= -3.1052 ZX= -1.6824
XY= -3.8509 YY= 23.6113 ZY= 0.2877
XZ= -1.4315 YZ= -0.2628 ZZ= 24.8694
Eigenvalues: 20.6752 24.6607 28.5071

Isomer 1 (conformer 3)

1 C Isotropic = 57.9614 Anisotropy = 143.1544
XX= 17.7614 YX= 18.6162 ZX= -44.8846
XY= 19.3923 YY= 140.2319 ZY= 41.4025
XZ= -48.0745 YZ= 43.0913 ZZ= 15.8909
Eigenvalues: -40.2785 60.7650 153.3977
2 C Isotropic = 47.5524 Anisotropy = 113.3946
XX= -30.1758 YX= -2.9677 ZX= 29.6994
XY= -6.1311 YY= 117.3452 ZY= 20.0703
XZ= 32.0816 YZ= 19.0864 ZZ= 55.4876
Eigenvalues: -40.8419 60.3502 123.1488
3 C Isotropic = 69.6336 Anisotropy = 125.5494
XX= 55.9076 YX= -3.1542 ZX= 23.1305
XY= -4.0638 YY= 140.6044 ZY= 42.3666
XZ= 27.6601 YZ= 41.7788 ZZ= 12.3889
Eigenvalues: -9.9646 65.5323 153.3332
4 C Isotropic = 47.2434 Anisotropy = 140.8074
XX= 5.5690 YX= 13.4297 ZX= -26.5581
XY= 12.8505 YY= 128.2702 ZY= 40.3991
XZ= -26.7645 YZ= 41.7336 ZZ= 7.8910
Eigenvalues: -29.4646 30.0798 141.1150
5 C Isotropic = 59.5066 Anisotropy = 160.1696
XX= -1.7069 YX= 3.1681 ZX= 12.6283
XY= 1.9134 YY= 153.9196 ZY= 40.7027
XZ= 16.8489 YZ= 41.5500 ZZ= 26.3071
Eigenvalues: -9.5417 21.7752 166.2863
6 C Isotropic = 60.7698 Anisotropy = 164.8981
XX= 46.0353 YX= 1.9103 ZX= 9.3423
XY= 9.1950 YY= 153.3079 ZY= 56.1794
XZ= 7.5785 YZ= 56.3664 ZZ= -17.0338
Eigenvalues: -34.4723 46.0798 170.7019
7 N Isotropic = 115.1219 Anisotropy = 84.7849
XX= 128.2786 YX= 3.3992 ZX= -8.2427
XY= -0.1012 YY= 161.3282 ZY= 33.7553
XZ= -4.9563 YZ= 35.3916 ZZ= 55.7589
Eigenvalues: 44.8903 128.8302 171.6452
8 C Isotropic = 61.0543 Anisotropy = 117.2839
XX= -7.5524 YX= 3.2651 ZX= 4.4577
XY= -2.3837 YY= 129.6473 ZY= 30.6712
XZ= 11.0641 YZ= 23.9138 ZZ= 61.0678
Eigenvalues: -8.4718 52.3910 139.2436
9 C Isotropic = 76.1682 Anisotropy = 108.2609
XX= 24.4934 YX= -1.9942 ZX= 23.2714
XY= -1.3300 YY= 140.4484 ZY= 25.8082
XZ= 14.1441 YZ= 25.4913 ZZ= 63.5629
Eigenvalues: 15.9068 64.2557 148.3422
10 C Isotropic = 36.6683 Anisotropy = 85.3295
XX= 58.1306 YX= 11.3272 ZX= 1.1131
XY= 5.9989 YY= 65.8135 ZY= 51.0027
XZ= 0.1396 YZ= 53.6477 ZZ= -13.9391
Eigenvalues: -39.9611 56.4114 93.5546
11 Br Isotropic = 1896.8298 Anisotropy = 1575.3096
XX= 2836.8913 YX= 55.3441 ZX= -382.8903
XY= 46.0210 YY= 1339.1729 ZY= -45.8253

XZ= -402.8312 YZ= -38.5293 ZZ= 1514.4253
Eigenvalues: 1327.5433 1415.9100 2947.0362
12 C Isotropic = 62.5002 Anisotropy = 52.6442
XX= 68.8486 YX= 17.9523 ZX= -23.3185
XY= 33.8478 YY= 69.1856 ZY= 11.2740
XZ= -40.1522 YZ= 29.6017 ZZ= 49.4666
Eigenvalues: 8.9066 80.9977 97.5964
13 N Isotropic = -21.5086 Anisotropy = 304.0657
XX= -45.4748 YX= 47.9127 ZX= 26.9489
XY= 64.9642 YY= 92.6257 ZY= 140.8911
XZ= 1.9101 YZ= 146.9356 ZZ= -111.6767
Eigenvalues: -187.2964 -58.4312 181.2019
14 C Isotropic = 30.0628 Anisotropy = 76.4228
XX= 35.1882 YX= -3.4323 ZX= 32.3655
XY= -3.1001 YY= 61.9839 ZY= 38.5256
XZ= 40.3309 YZ= 33.3477 ZZ= -6.9835
Eigenvalues: -38.8316 48.0088 81.0114
15 O Isotropic = 34.2821 Anisotropy = 220.7431
XX= 6.2237 YX= 53.2510 ZX= -15.7557
XY= 38.9267 YY= 120.9905 ZY= 104.5484
XZ= 32.1368 YZ= 90.4271 ZZ= -24.3677
Eigenvalues: -75.7040 -2.8938 181.4442
16 C Isotropic = 62.5950 Anisotropy = 97.6552
XX= 30.9024 YX= 34.9729 ZX= -16.4066
XY= 31.7395 YY= 99.3117 ZY= 39.2383
XZ= -10.1014 YZ= 37.8359 ZZ= 57.5708
Eigenvalues: 2.0529 58.0335 127.6984
17 N Isotropic = 99.6519 Anisotropy = 121.1623
XX= 43.0233 YX= 13.7534 ZX= 48.4956
XY= 14.1278 YY= 162.3586 ZY= 28.3800
XZ= 47.8405 YZ= 30.1167 ZZ= 93.5739
Eigenvalues: 13.8281 104.7009 180.4268
18 C Isotropic = 63.9742 Anisotropy = 115.5489
XX= 45.4266 YX= 34.3312 ZX= -15.9906
XY= 36.7802 YY= 103.9402 ZY= 54.0348
XZ= -21.5322 YZ= 54.9872 ZZ= 42.5558
Eigenvalues: -11.1092 62.0250 141.0068
19 C Isotropic = 70.8735 Anisotropy = 137.1660
XX= 61.1960 YX= 17.6028 ZX= 20.5189
XY= 17.4452 YY= 126.2999 ZY= 62.4974
XZ= 22.1026 YZ= 62.4282 ZZ= 25.1246
Eigenvalues: -6.7967 57.0998 162.3175
20 C Isotropic = 69.6052 Anisotropy = 142.6356
XX= 3.3746 YX= 36.1662 ZX= 16.5622
XY= 35.8280 YY= 134.1418 ZY= 41.4372
XZ= 15.9373 YZ= 42.2297 ZZ= 71.2994
Eigenvalues: -6.3198 50.4399 164.6956
21 I Isotropic = 3721.7838 Anisotropy = 1962.1612
XX= 3998.0559 YX= -577.7705 ZX= 772.5212
XY= -780.2420 YY= 3708.7741 ZY= -426.6798
XZ= 801.1332 YZ= -380.8779 ZZ= 3458.5215
Eigenvalues: 2886.8261 3248.6340 5029.8913
22 H Isotropic = 24.1215 Anisotropy = 10.3903
XX= 26.9503 YX= 0.7563 ZX= -4.0276
XY= 0.9168 YY= 18.7828 ZY= -2.6355

XZ= -3.5009 YZ= -2.6406 ZZ= 26.6314
Eigenvalues: 17.9666 23.3495 31.0484
23 H Isotropic = 24.1047 Anisotropy = 10.3002
XX= 30.3401 YX= -1.2223 ZX= 2.0501
XY= -1.0045 YY= 18.1656 ZY= -1.9011
XZ= 1.4368 YZ= -2.0432 ZZ= 23.8085
Eigenvalues: 17.5209 23.8217 30.9715
24 H Isotropic = 23.3037 Anisotropy = 10.6707
XX= 30.3169 YX= -0.3872 ZX= -0.7504
XY= 0.2635 YY= 17.0482 ZY= -3.1855
XZ= -0.9791 YZ= -2.6818 ZZ= 22.5459
Eigenvalues: 15.7657 23.7279 30.4175
25 H Isotropic = 24.0251 Anisotropy = 9.4198
XX= 26.3781 YX= -0.6089 ZX= -0.1970
XY= -0.5506 YY= 16.6854 ZY= -4.2004
XZ= -1.0088 YZ= -4.0399 ZZ= 29.0117
Eigenvalues: 15.3866 26.3837 30.3050
26 H Isotropic = 23.3784 Anisotropy = 13.0101
XX= 27.4072 YX= -0.7256 ZX= -6.0755
XY= -0.6993 YY= 15.7029 ZY= -1.4511
XZ= -3.5055 YZ= -2.3777 ZZ= 27.0251
Eigenvalues: 15.1788 22.9046 32.0518
27 H Isotropic = 23.0874 Anisotropy = 9.0106
XX= 26.1043 YX= -1.5503 ZX= -2.5762
XY= -1.3729 YY= 17.5974 ZY= -5.4363
XZ= -2.4568 YZ= -4.8389 ZZ= 25.5606
Eigenvalues: 14.5631 25.6047 29.0945
28 H Isotropic = 24.6830 Anisotropy = 3.6772
XX= 25.8125 YX= -1.3545 ZX= 0.2648
XY= -0.9292 YY= 22.4841 ZY= -2.6142
XZ= -0.6988 YZ= -2.2029 ZZ= 25.7525
Eigenvalues: 20.9528 25.9617 27.1345
29 H Isotropic = 25.1183 Anisotropy = 2.4675
XX= 26.0153 YX= -0.9012 ZX= -0.0920
XY= -0.7883 YY= 23.4910 ZY= -1.8760
XZ= -0.6126 YZ= -1.5547 ZZ= 25.8486
Eigenvalues: 22.3609 26.2307 26.7633
30 H Isotropic = 24.3218 Anisotropy = 5.5162
XX= 24.2777 YX= -0.7168 ZX= -0.4841
XY= -0.9394 YY= 22.1382 ZY= -2.8922
XZ= -0.1608 YZ= -2.9336 ZZ= 26.5494
Eigenvalues: 20.4836 24.4825 27.9993

Isomer 1 (conformer 4)

1 C Isotropic = 58.1741 Anisotropy = 144.2846
XX= 10.1639 YX= -26.3843 ZX= -47.9463
XY= -28.0713 YY= 148.3370 ZY= 0.0214
XZ= -52.3363 YZ= 1.7391 ZZ= 16.0213
Eigenvalues: -39.1400 59.2983 154.3638
2 C Isotropic = 46.9202 Anisotropy = 113.4344
XX= -13.2437 YX= -32.2751 ZX= 35.6815
XY= -35.9981 YY= 113.1982 ZY= 17.2409
XZ= 39.2443 YZ= 16.3568 ZZ= 40.8059
Eigenvalues: -41.7517 59.9691 122.5431
3 C Isotropic = 70.2706 Anisotropy = 124.9183
XX= 66.3094 YX= -19.1239 ZX= 9.7501
XY= -19.4704 YY= 147.0616 ZY= 22.0838
XZ= 16.2416 YZ= 20.6617 ZZ= -2.5592
Eigenvalues: -8.8508 66.1132 153.5495
4 C Isotropic = 47.3865 Anisotropy = 141.4350
XX= 0.3761 YX= -23.8101 ZX= -32.1592
XY= -26.3373 YY= 135.2766 ZY= 9.9324
XZ= -33.5499 YZ= 9.9517 ZZ= 6.5067
Eigenvalues: -30.4490 30.9319 141.6765
5 C Isotropic = 57.7039 Anisotropy = 165.1827
XX= 5.2036 YX= -33.7366 ZX= 8.0213
XY= -33.6487 YY= 159.6992 ZY= 14.0539
XZ= 10.5671 YZ= 16.8006 ZZ= 8.2088
Eigenvalues: -10.3576 15.6436 167.8257
6 C Isotropic = 58.9028 Anisotropy = 175.3382
XX= 42.0429 YX= -26.3755 ZX= -7.0225
XY= -20.4490 YY= 170.3695 ZY= 15.6526
XZ= -9.5342 YZ= 14.9186 ZZ= -35.7039
Eigenvalues: -37.3882 38.3017 175.7950
7 N Isotropic = 114.7083 Anisotropy = 87.8872
XX= 122.9915 YX= -8.0637 ZX= -24.5492
XY= -13.5043 YY= 169.4212 ZY= 7.0590
XZ= -17.1965 YZ= 10.5960 ZZ= 51.7121
Eigenvalues: 45.7830 125.0421 173.2997
8 C Isotropic = 60.7396 Anisotropy = 115.2451
XX= -6.2823 YX= -29.4260 ZX= 9.4447
XY= -29.4705 YY= 130.7862 ZY= 8.3819
XZ= 19.6561 YZ= 12.9614 ZZ= 57.7149
Eigenvalues: -16.0090 60.6581 137.5696
9 C Isotropic = 76.4554 Anisotropy = 106.7029
XX= 34.5184 YX= -23.4012 ZX= 30.2841
XY= -19.6592 YY= 142.6345 ZY= 13.9007
XZ= 24.8211 YZ= 14.0218 ZZ= 52.2133
Eigenvalues: 9.4955 72.2800 147.5907
10 C Isotropic = 38.9130 Anisotropy = 84.5547
XX= 16.8044 YX= 35.4075 ZX= 53.5866
XY= 29.0134 YY= 74.0007 ZY= -10.1208
XZ= 57.8885 YZ= -4.6529 ZZ= 25.9339
Eigenvalues: -41.8055 63.2618 95.2828
11 Br Isotropic = 1889.1697 Anisotropy = 1564.6783
XX= 2620.3822 YX= 328.9091 ZX= -511.6314
XY= 334.2029 YY= 1401.7024 ZY= -142.3606

XZ= -531.4164 YZ= -147.0955 ZZ= 1645.4244
Eigenvalues: 1316.1910 1419.0294 2932.2885
12 C Isotropic = 55.1296 Anisotropy = 49.3069
XX= 29.6426 YX= 50.4508 ZX= 3.6399
XY= 38.4009 YY= 49.6155 ZY= -1.2913
XZ= 15.7831 YZ= -15.6487 ZZ= 86.1308
Eigenvalues: -7.6725 85.0605 88.0009
13 N Isotropic = -22.8152 Anisotropy = 304.1049
XX= -57.8337 YX= 134.0525 ZX= 104.7856
XY= 121.6980 YY= 39.5382 ZY= 64.1610
XZ= 124.3194 YZ= 36.4235 ZZ= -50.1501
Eigenvalues: -188.2755 -60.0915 179.9214
14 C Isotropic = 27.4240 Anisotropy = 83.2138
XX= 36.9451 YX= 6.6542 ZX= 50.5957
XY= 22.5791 YY= 54.8796 ZY= 13.8879
XZ= 47.5044 YZ= 16.1358 ZZ= -9.5528
Eigenvalues: -40.8430 40.2151 82.8998
15 O Isotropic = 21.6771 Anisotropy = 215.3703
XX= 8.0428 YX= 77.3276 ZX= 80.0218
XY= 115.8378 YY= 52.1255 ZY= 24.4892
XZ= 57.2261 YZ= 58.7333 ZZ= 4.8630
Eigenvalues: -81.8206 -18.4053 165.2573
16 C Isotropic = 62.4517 Anisotropy = 98.1697
XX= 51.6531 YX= 53.4344 ZX= 15.7173
XY= 57.0358 YY= 65.8017 ZY= 23.3364
XZ= 10.8060 YZ= 27.5849 ZZ= 69.9002
Eigenvalues: 2.2646 57.1923 127.8981
17 N Isotropic = 100.0530 Anisotropy = 123.3151
XX= 130.6756 YX= 26.9757 ZX= 25.2981
XY= 27.5880 YY= 119.8588 ZY= 63.1036
XZ= 25.8918 YZ= 61.5385 ZZ= 49.6245
Eigenvalues: 12.5694 105.3265 182.2631
18 C Isotropic = 63.9288 Anisotropy = 116.4216
XX= 41.0664 YX= 66.3787 ZX= 26.8628
XY= 64.4271 YY= 75.4229 ZY= 20.2252
XZ= 31.1017 YZ= 15.8846 ZZ= 75.2971
Eigenvalues: -11.1760 61.4192 141.5432
19 C Isotropic = 70.8561 Anisotropy = 136.7870
XX= 62.6350 YX= 45.8923 ZX= 58.2800
XY= 46.9125 YY= 106.5066 ZY= 26.6195
XZ= 57.2296 YZ= 26.8373 ZZ= 43.4266
Eigenvalues: -6.5480 57.0688 162.0474
20 C Isotropic = 69.4311 Anisotropy = 144.0895
XX= 81.1197 YX= 60.0727 ZX= 15.7560
XY= 59.3273 YY= 78.9823 ZY= 59.6229
XZ= 16.6119 YZ= 59.6696 ZZ= 48.1914
Eigenvalues: -6.9284 49.7310 165.4908
21 I Isotropic = 3790.3258 Anisotropy = 1984.5601
XX= 4173.7633 YX= -974.7420 ZX= 238.7423
XY= -887.0780 YY= 4186.1443 ZY= 24.5588
XZ= 136.3432 YZ= 145.3950 ZZ= 3011.0699
Eigenvalues: 2901.5863 3356.0254 5113.3659
22 H Isotropic = 24.1366 Anisotropy = 10.4364
XX= 25.4772 YX= 2.3705 ZX= -3.7138
XY= 2.6875 YY= 19.0999 ZY= -2.2091

XZ= -3.0354 YZ= -2.0724 ZZ= 27.8328
Eigenvalues: 18.1134 23.2023 31.0942
23 H Isotropic = 24.1425 Anisotropy = 9.7053
XX= 29.9745 YX= 2.2699 ZX= 1.5303
XY= 2.3547 YY= 18.3775 ZY= -0.6454
XZ= 1.0305 YZ= -0.8080 ZZ= 24.0756
Eigenvalues: 17.7860 24.0288 30.6127
24 H Isotropic = 23.5764 Anisotropy = 10.9538
XX= 27.6334 YX= 4.2968 ZX= -1.1673
XY= 5.5706 YY= 21.8175 ZY= -2.6415
XZ= -0.5708 YZ= -2.3656 ZZ= 21.2782
Eigenvalues: 17.9793 21.8709 30.8789
25 H Isotropic = 23.8631 Anisotropy = 9.8930
XX= 25.1917 YX= 1.2643 ZX= 1.3010
XY= 1.2533 YY= 16.3383 ZY= -2.0985
XZ= 0.4849 YZ= -2.0294 ZZ= 30.0592
Eigenvalues: 15.8317 25.2991 30.4584
26 H Isotropic = 24.3035 Anisotropy = 5.9807
XX= 25.0098 YX= 0.1133 ZX= -0.1373
XY= 0.4937 YY= 19.7284 ZY= -0.0024
XZ= 1.1697 YZ= -1.2195 ZZ= 28.1722
Eigenvalues: 19.6627 24.9571 28.2906
27 H Isotropic = 23.2795 Anisotropy = 7.4497
XX= 23.2018 YX= -3.8207 ZX= -3.4515
XY= -4.5797 YY= 20.8029 ZY= -3.0054
XZ= -3.4868 YZ= -3.4161 ZZ= 25.8338
Eigenvalues: 15.5220 26.0705 28.2460
28 H Isotropic = 24.7401 Anisotropy = 3.6852
XX= 25.3244 YX= -2.0787 ZX= -1.8302
XY= -2.6959 YY= 23.8318 ZY= -0.8117
XZ= -0.9450 YZ= -1.5344 ZZ= 25.0642
Eigenvalues: 21.2513 25.7721 27.1969
29 H Isotropic = 25.1544 Anisotropy = 2.5147
XX= 25.3724 YX= -1.4662 ZX= -1.3216
XY= -1.9065 YY= 24.5200 ZY= -0.8193
XZ= -0.9560 YZ= -1.0821 ZZ= 25.5709
Eigenvalues: 22.5139 26.1185 26.8309
30 H Isotropic = 24.2576 Anisotropy = 5.5745
XX= 25.3561 YX= -2.2679 ZX= -2.4359
XY= -2.0893 YY= 22.5856 ZY= -0.6909
XZ= -2.6394 YZ= -0.4077 ZZ= 24.8310
Eigenvalues: 20.5842 24.2146 27.9739

Isomer 2 (conformer 1)

1 C Isotropic = 56.5022 Anisotropy = 145.9495
XX= -37.6459 YX= 0.0000 ZX= -21.9816
XY= 0.0000 YY= 153.8019 ZY= 0.0000
XZ= -18.1786 YZ= 0.0000 ZZ= 53.3507
Eigenvalues: -41.8800 57.5848 153.8019
2 C Isotropic = 46.4931 Anisotropy = 114.0605
XX= 56.7450 YX= 0.0000 ZX= -15.5558
XY= 0.0000 YY= 122.5334 ZY= 0.0000
XZ= -19.6673 YZ= 0.0000 ZZ= -39.7991
Eigenvalues: -42.9115 59.8574 122.5334
3 C Isotropic = 70.2674 Anisotropy = 125.2335
XX= 34.7348 YX= 0.0000 ZX= 39.4155
XY= 0.0000 YY= 153.7564 ZY= 0.0000
XZ= 34.5955 YZ= 0.0000 ZZ= 22.3109
Eigenvalues: -9.0004 66.0461 153.7564
4 C Isotropic = 46.2883 Anisotropy = 138.4198
XX= -28.1349 YX= 0.0000 ZX= -13.8366
XY= 0.0000 YY= 138.5682 ZY= 0.0000
XZ= -13.2993 YZ= 0.0000 ZZ= 28.4317
Eigenvalues: -31.2209 31.5177 138.5682
5 C Isotropic = 59.3031 Anisotropy = 164.1988
XX= 21.7415 YX= 0.0000 ZX= -0.2538
XY= 0.0000 YY= 168.7690 ZY= 0.0000
XZ= -0.3933 YZ= 0.0000 ZZ= -12.6010
Eigenvalues: -12.6041 21.7445 168.7690
6 C Isotropic = 57.8292 Anisotropy = 177.7378
XX= -17.7989 YX= 0.0000 ZX= 30.3502
XY= 0.0000 YY= 176.3211 ZY= 0.0000
XZ= 34.9423 YZ= 0.0000 ZZ= 14.9655
Eigenvalues: -37.9428 35.1094 176.3211
7 N Isotropic = 115.4866 Anisotropy = 84.7218
XX= 60.2834 YX= 0.0000 ZX= 33.3681
XY= 0.0000 YY= 171.9678 ZY= 0.0000
XZ= 21.9501 YZ= 0.0000 ZZ= 114.2086
Eigenvalues: 48.6195 125.8725 171.9678
8 C Isotropic = 62.6919 Anisotropy = 114.1345
XX= 47.3982 YX= 0.0000 ZX= -15.9548
XY= 0.0000 YY= 138.7816 ZY= 0.0000
XZ= -33.5038 YZ= 0.0000 ZZ= 1.8958
Eigenvalues: -8.9558 58.2499 138.7816
9 C Isotropic = 75.0772 Anisotropy = 106.3357
XX= 63.4964 YX= 0.0000 ZX= -9.7278
XY= 0.0000 YY= 145.9677 ZY= 0.0000
XZ= -1.6298 YZ= 0.0000 ZZ= 15.7676
Eigenvalues: 15.1012 64.1627 145.9677
10 C Isotropic = 27.8932 Anisotropy = 75.7767
XX= 40.7920 YX= 0.0000 ZX= -17.4605
XY= 0.0000 YY= 78.4110 ZY= 0.0000
XZ= -27.8314 YZ= 0.0000 ZZ= -35.5234
Eigenvalues: -41.7374 47.0060 78.4110
11 Br Isotropic = 1888.8850 Anisotropy = 1579.9278
XX= 1498.0880 YX= 0.0000 ZX= 330.4543
XY= 0.0000 YY= 1306.5173 ZY= 0.0000

XZ= 349.8414 YZ= 0.0000 ZZ= 2862.0497
Eigenvalues: 1306.5173 1417.9675 2942.1702
12 O Isotropic = 39.1253 Anisotropy = 200.4816
XX= -9.9388 YX= 0.0000 ZX= 63.2759
XY= 0.0000 YY= 172.7797 ZY= 0.0000
XZ= 3.9719 YZ= 0.0000 ZZ= -45.4649
Eigenvalues: -65.7294 10.3256 172.7797
13 C Isotropic = 40.0663 Anisotropy = 89.6828
XX= 50.9047 YX= 0.0000 ZX= 23.2787
XY= 0.0000 YY= 99.8549 ZY= 0.0000
XZ= 23.1684 YZ= 0.0000 ZZ= -30.5606
Eigenvalues: -36.7159 57.0600 99.8549
14 C Isotropic = 64.9465 Anisotropy = 40.1698
XX= 47.7140 YX= 0.0000 ZX= 26.0181
XY= 0.0000 YY= 88.9466 ZY= 0.0000
XZ= 50.8324 YZ= 0.0000 ZZ= 58.1790
Eigenvalues: 14.1666 88.9466 91.7264
15 N Isotropic = -28.5742 Anisotropy = 308.7738
XX= -87.3942 YX= 0.0000 ZX= 31.7579
XY= 0.0000 YY= 177.2749 ZY= 0.0000
XZ= 50.9641 YZ= 0.0000 ZZ= -175.6034
Eigenvalues: -191.9633 -71.0344 177.2749
16 C Isotropic = 63.1304 Anisotropy = 102.3719
XX= 16.1897 YX= 0.0000 ZX= -26.8155
XY= 0.0000 YY= 131.3783 ZY= 0.0000
XZ= -17.6149 YZ= 0.0000 ZZ= 41.8232
Eigenvalues: 3.3592 54.6537 131.3783
17 N Isotropic = 100.9647 Anisotropy = 114.7042
XX= 54.5244 YX= 0.0000 ZX= 49.3057
XY= 0.0000 YY= 177.4342 ZY= 0.0000
XZ= 40.7952 YZ= 0.0000 ZZ= 70.9355
Eigenvalues: 16.9383 108.5216 177.4342
18 C Isotropic = 65.6843 Anisotropy = 114.8346
XX= 25.5087 YX= 0.0000 ZX= -33.0553
XY= 0.0000 YY= 142.2407 ZY= 0.0000
XZ= -42.9428 YZ= 0.0000 ZZ= 29.3035
Eigenvalues: -10.6403 65.4525 142.2407
19 C Isotropic = 71.2908 Anisotropy = 135.5095
XX= 59.8399 YX= 0.0000 ZX= -4.8860
XY= 0.0000 YY= 161.6305 ZY= 0.0000
XZ= -0.2087 YZ= 0.0000 ZZ= -7.5979
Eigenvalues: -7.6940 59.9360 161.6305
20 C Isotropic = 71.8758 Anisotropy = 138.0090
XX= 4.5802 YX= 0.0000 ZX= 11.0005
XY= 0.0000 YY= 163.8818 ZY= 0.0000
XZ= 12.9483 YZ= 0.0000 ZZ= 47.1654
Eigenvalues: 1.4441 50.3015 163.8818
21 I Isotropic = 3670.1979 Anisotropy = 1962.9815
XX= 4506.4117 YX= 0.0000 ZX= -867.4320
XY= 0.0000 YY= 3195.1294 ZY= 0.0000
XZ= -908.9475 YZ= 0.0000 ZZ= 3309.0527
Eigenvalues: 2836.6121 3195.1294 4978.8523
22 H Isotropic = 24.0202 Anisotropy = 10.4828
XX= 23.9220 YX= 0.0000 ZX= -2.3490
XY= 0.0000 YY= 17.9743 ZY= 0.0000
XZ= -2.5435 YZ= 0.0000 ZZ= 30.1644
Eigenvalues: 17.9743 23.0776 31.0088

23 H Isotropic = 24.2251 Anisotropy = 10.0281
XX= 27.6098 YX= 0.0000 ZX= 3.1084
XY= 0.0000 YY= 17.8047 ZY= 0.0000
XZ= 3.8331 YZ= 0.0000 ZZ= 27.2609
Eigenvalues: 17.8047 23.9602 30.9105
24 H Isotropic = 22.8347 Anisotropy = 10.5517
XX= 23.7051 YX= 0.0000 ZX= 1.6622
XY= 0.0000 YY= 15.5275 ZY= 0.0000
XZ= 2.1766 YZ= 0.0000 ZZ= 29.2715
Eigenvalues: 15.5275 23.1075 29.8692
25 H Isotropic = 24.0353 Anisotropy = 9.4802
XX= 29.1953 YX= 0.0000 ZX= -2.2366
XY= 0.0000 YY= 15.7724 ZY= 0.0000
XZ= -1.6272 YZ= 0.0000 ZZ= 27.1381
Eigenvalues: 15.7724 25.9780 30.3554
26 H Isotropic = 24.0176 Anisotropy = 6.2860
XX= 26.5369 YX= 0.0000 ZX= -0.3652
XY= 0.0000 YY= 18.2783 ZY= 0.0000
XZ= -2.1821 YZ= 0.0000 ZZ= 27.2376
Eigenvalues: 18.2783 25.5662 28.2082
27 H Isotropic = 23.4066 Anisotropy = 7.9717
XX= 27.1711 YX= 0.0000 ZX= -0.8598
XY= 0.0000 YY= 14.8444 ZY= 0.0000
XZ= -0.9301 YZ= 0.0000 ZZ= 28.2043
Eigenvalues: 14.8444 26.6544 28.7210
28 H Isotropic = 24.7076 Anisotropy = 3.6674
XX= 26.4845 YX= 0.0000 ZX= 1.2954
XY= 0.0000 YY= 21.1378 ZY= 0.0000
XZ= 0.0244 YZ= 0.0000 ZZ= 26.5006
Eigenvalues: 21.1378 25.8326 27.1525
29 H Isotropic = 25.0900 Anisotropy = 2.9985
XX= 26.5048 YX= 0.0000 ZX= 0.7779
XY= 0.0000 YY= 22.1295 ZY= 0.0000
XZ= 0.2513 YZ= 0.0000 ZZ= 26.6359
Eigenvalues: 22.1295 26.0516 27.0890
30 H Isotropic = 24.2723 Anisotropy = 11.9313
XX= 25.9709 YX= 0.0000 ZX= 4.6793
XY= 0.0000 YY= 17.7182 ZY= 0.0000
XZ= 4.1261 YZ= 0.0000 ZZ= 29.1279
Eigenvalues: 17.7182 22.8723 32.2265

Isomer 2 (conformer 2)

1 C Isotropic = 57.3171 Anisotropy = 144.4023
XX= -39.4673 YX= -2.5848 ZX= -14.2186
XY= -2.9705 YY= 153.5447 ZY= 0.0453
XZ= -10.5192 YZ= 0.0746 ZZ= 57.8739
Eigenvalues: -41.0532 59.4192 153.5853
2 C Isotropic = 47.5282 Anisotropy = 113.7603
XX= 53.5511 YX= -0.9695 ZX= -23.4708
XY= -0.8954 YY= 123.3559 ZY= -0.2410
XZ= -27.2132 YZ= -0.2019 ZZ= -34.3223
Eigenvalues: -41.1081 60.3244 123.3684
3 C Isotropic = 68.7197 Anisotropy = 126.9948
XX= 38.9397 YX= -1.6636 ZX= 37.3446
XY= -1.4318 YY= 153.3616 ZY= 0.5661
XZ= 33.1640 YZ= 0.8279 ZZ= 13.8577
Eigenvalues: -11.0327 63.8088 153.3829
4 C Isotropic = 46.5671 Anisotropy = 137.6626
XX= -28.9297 YX= -2.1203 ZX= -7.0242
XY= -2.1772 YY= 138.3138 ZY= 0.1980
XZ= -6.3973 YZ= 0.2135 ZZ= 30.3171
Eigenvalues: -29.7068 31.0659 138.3422
5 C Isotropic = 59.8536 Anisotropy = 163.6972
XX= 21.9680 YX= -1.9246 ZX= -2.1440
XY= -1.8422 YY= 168.9589 ZY= 0.7158
XZ= -1.7882 YZ= 0.4317 ZZ= -11.3663
Eigenvalues: -11.4830 22.0587 168.9850
6 C Isotropic = 61.0613 Anisotropy = 165.2417
XX= -3.4923 YX= -2.4542 ZX= 36.3647
XY= -2.1652 YY= 171.1895 ZY= 1.2951
XZ= 40.7451 YZ= 0.9102 ZZ= 15.4867
Eigenvalues: -33.7388 45.7003 171.2225
7 N Isotropic = 112.9050 Anisotropy = 89.8285
XX= 59.1195 YX= -1.6092 ZX= 38.5190
XY= -1.8523 YY= 172.7643 ZY= 0.4620
XZ= 27.1633 YZ= 0.5260 ZZ= 106.8312
Eigenvalues: 42.3603 123.5640 172.7906
8 C Isotropic = 58.6395 Anisotropy = 119.6653
XX= 37.8552 YX= -1.2753 ZX= -22.7557
XY= -1.4698 YY= 138.3940 ZY= 0.6382
XZ= -35.6856 YZ= -0.0689 ZZ= -0.3308
Eigenvalues: -16.1443 53.6463 138.4163
9 C Isotropic = 75.4502 Anisotropy = 103.8370
XX= 63.4110 YX= -1.0108 ZX= -14.2545
XY= -1.4699 YY= 144.6554 ZY= -0.1187
XZ= -7.4365 YZ= 0.2699 ZZ= 18.2841
Eigenvalues: 15.8125 65.8631 144.6748
10 C Isotropic = 27.3054 Anisotropy = 73.6412
XX= -19.9624 YX= 0.5961 ZX= 32.8477
XY= -0.1336 YY= 76.3983 ZY= -0.6750
XZ= 43.3562 YZ= 0.1883 ZZ= 25.4804
Eigenvalues: -41.6043 47.1211 76.3995
11 Br Isotropic = 1894.2209 Anisotropy = 1571.0305
XX= 1568.5158 YX= 3.4973 ZX= 450.9757
XY= 1.8564 YY= 1325.5648 ZY= 4.4530
XZ= 465.6231 YZ= 5.5051 ZZ= 2788.5821
Eigenvalues: 1325.5353 1415.5528 2941.5745
12 O Isotropic = 33.3584 Anisotropy = 216.7478
XX= -11.7582 YX= 1.0883 ZX= -1.0124

XY= 1.5750 YY= 177.8327 ZY= 1.5436
XZ= 48.9511 YZ= 1.8959 ZZ= -65.9995
Eigenvalues: -75.0787 -2.7031 177.8569
13 C Isotropic = 39.2039 Anisotropy = 89.4104
XX= 30.8515 YX= 0.2748 ZX= 39.5147
XY= 0.9282 YY= 98.7969 ZY= 0.7636
XZ= 41.4952 YZ= 0.2549 ZZ= -12.0366
Eigenvalues: -36.4238 55.2248 98.8109
14 C Isotropic = 65.0978 Anisotropy = 38.5529
XX= 90.3392 YX= -0.0138 ZX= 8.1735
XY= -0.6854 YY= 89.9645 ZY= 1.0985
XZ= -17.3132 YZ= 0.2964 ZZ= 14.9898
Eigenvalues: 14.7076 89.7862 90.7997
15 N Isotropic = -24.5291 Anisotropy = 299.0726
XX= -88.5286 YX= 1.6974 ZX= 71.4233
XY= 0.9565 YY= 174.8234 ZY= 2.9642
XZ= 36.8677 YZ= 1.8915 ZZ= -159.8821
Eigenvalues: -189.0542 -59.3857 174.8526
16 C Isotropic = 63.0629 Anisotropy = 102.3942
XX= 6.5070 YX= 2.5670 ZX= -8.5155
XY= 2.4937 YY= 131.1865 ZY= 2.8231
XZ= -17.8614 YZ= 2.9643 ZZ= 51.4953
Eigenvalues: 2.8460 55.0171 131.3257
17 N Isotropic = 101.4733 Anisotropy = 111.2835
XX= 110.2680 YX= 1.4357 ZX= -11.4628
XY= 1.2052 YY= 175.4567 ZY= 5.2570
XZ= -2.5606 YZ= 5.6014 ZZ= 18.6952
Eigenvalues: 17.9684 110.7892 175.6623
18 C Isotropic = 65.5280 Anisotropy = 114.5865
XX= -10.3401 YX= 2.7251 ZX= -7.3631
XY= 2.8946 YY= 141.7617 ZY= 3.2554
XZ= 3.0651 YZ= 2.5112 ZZ= 65.1623
Eigenvalues: -10.4561 65.1211 141.9189
19 C Isotropic = 71.2451 Anisotropy = 135.6032
XX= 22.4825 YX= 1.0926 ZX= 35.6352
XY= 1.3316 YY= 161.5111 ZY= 3.5587
XZ= 30.5602 YZ= 3.7602 ZZ= 29.7419
Eigenvalues: -7.1980 59.2862 161.6473
20 C Isotropic = 72.2192 Anisotropy = 137.2200
XX= 37.6085 YX= 2.7717 ZX= -19.4180
XY= 3.3084 YY= 163.4975 ZY= 4.6448
XZ= -22.3033 YZ= 4.9817 ZZ= 15.5517
Eigenvalues: 2.7820 50.1764 163.6992
21 I Isotropic = 3716.7557 Anisotropy = 1922.8734
XX= 3036.1905 YX= -2.8021 ZX= 570.4025
XY= 9.2107 YY= 3298.7589 ZY= 7.2056
XZ= 629.3104 YZ= -8.2605 ZZ= 4815.3177
Eigenvalues: 2852.8138 3298.7820 4998.6714
22 H Isotropic = 24.0624 Anisotropy = 10.5530
XX= 23.5615 YX= 0.0675 ZX= -1.6395
XY= 0.0639 YY= 17.9652 ZY= -0.0109
XZ= -1.9898 YZ= -0.0470 ZZ= 30.6607
Eigenvalues: 17.9644 23.1251 31.0978
23 H Isotropic = 24.1059 Anisotropy = 10.1032
XX= 28.1334 YX= 0.1207 ZX= 3.0875
XY= 0.1495 YY= 17.6618 ZY= 0.0009
XZ= 3.7502 YZ= 0.0323 ZZ= 26.5226
Eigenvalues: 17.6600 23.8164 30.8414

24 H Isotropic = 23.3212 Anisotropy = 10.5083
XX= 24.8237 YX= 0.0426 ZX= 2.0248
XY= 0.0392 YY= 15.7712 ZY= 0.1065
XZ= 2.5659 YZ= 0.0482 ZZ= 29.3688
Eigenvalues: 15.7707 23.8663 30.3268
25 H Isotropic = 23.9009 Anisotropy = 9.3835
XX= 28.6974 YX= 0.1744 ZX= -2.2789
XY= 0.1333 YY= 15.6646 ZY= -0.0577
XZ= -1.7715 YZ= -0.0608 ZZ= 27.3406
Eigenvalues: 15.6627 25.8834 30.1565
26 H Isotropic = 23.6088 Anisotropy = 6.2586
XX= 25.6732 YX= 0.0659 ZX= -0.3436
XY= 0.1775 YY= 18.0713 ZY= -0.0669
XZ= -2.0815 YZ= -0.0622 ZZ= 27.0819
Eigenvalues: 18.0692 24.9761 27.7812
27 H Isotropic = 23.2053 Anisotropy = 9.1660
XX= 26.5209 YX= -0.1718 ZX= -0.9920
XY= -0.3365 YY= 14.0906 ZY= -0.3840
XZ= -0.8590 YZ= -0.3360 ZZ= 29.0046
Eigenvalues: 14.0757 26.2243 29.3160
28 H Isotropic = 24.7263 Anisotropy = 3.6390
XX= 27.1435 YX= -0.0637 ZX= -0.7836
XY= -0.1092 YY= 20.8394 ZY= -0.0707
XZ= 0.6103 YZ= -0.1484 ZZ= 26.1959
Eigenvalues: 20.8360 26.1906 27.1523
29 H Isotropic = 25.1040 Anisotropy = 3.0029
XX= 27.0935 YX= -0.0448 ZX= -0.3456
XY= -0.0224 YY= 21.9963 ZY= -0.1063
XZ= 0.1359 YZ= -0.1042 ZZ= 26.2224
Eigenvalues: 21.9934 26.2127 27.1060
30 H Isotropic = 24.2556 Anisotropy = 11.7126
XX= 31.8130 YX= 0.0459 ZX= -1.6480
XY= 0.0277 YY= 17.4933 ZY= -0.1790
XZ= -1.2895 YZ= -0.1329 ZZ= 23.4603
Eigenvalues: 17.4893 23.2134 32.0640

Isomer 2 (conformer 3)

1 C Isotropic = 56.9299 Anisotropy = 145.2223
XX= -39.9074 YX= 0.0000 ZX= -15.1370
XY= 0.0000 YY= 153.7448 ZY= 0.0000
XZ= -11.3608 YZ= 0.0000 ZZ= 56.9523
Eigenvalues: -41.6869 58.7318 153.7448
2 C Isotropic = 47.2120 Anisotropy = 113.7135
XX= 53.6304 YX= 0.0000 ZX= -22.9408
XY= 0.0000 YY= 123.0210 ZY= 0.0000
XZ= -26.5067 YZ= 0.0000 ZZ= -35.0155
Eigenvalues: -41.4448 60.0597 123.0210
3 C Isotropic = 69.1441 Anisotropy = 126.3907
XX= 38.6484 YX= 0.0000 ZX= 37.6384
XY= 0.0000 YY= 153.4045 ZY= 0.0000
XZ= 33.6215 YZ= 0.0000 ZZ= 15.3794
Eigenvalues: -10.4675 64.4953 153.4045
4 C Isotropic = 46.4976 Anisotropy = 137.6989
XX= -29.2788 YX= 0.0000 ZX= -8.0333
XY= 0.0000 YY= 138.2968 ZY= 0.0000
XZ= -7.3384 YZ= 0.0000 ZZ= 30.4748
Eigenvalues: -30.2516 31.4475 138.2968
5 C Isotropic = 59.6747 Anisotropy = 164.3128
XX= 22.2616 YX= 0.0000 ZX= -2.4709
XY= 0.0000 YY= 169.2166 ZY= 0.0000
XZ= -1.4054 YZ= 0.0000 ZZ= -12.4541
Eigenvalues: -12.5620 22.3695 169.2166
6 C Isotropic = 59.7304 Anisotropy = 169.8394
XX= -7.3018 YX= 0.0000 ZX= 34.2424
XY= 0.0000 YY= 172.9567 ZY= 0.0000
XZ= 39.0125 YZ= 0.0000 ZZ= 13.5363
Eigenvalues: -34.9633 41.1978 172.9567
7 N Isotropic = 112.8531 Anisotropy = 89.6108
XX= 58.2077 YX= 0.0000 ZX= 38.1413
XY= 0.0000 YY= 172.5937 ZY= 0.0000
XZ= 26.6045 YZ= 0.0000 ZZ= 107.7581
Eigenvalues: 42.2175 123.7482 172.5937
8 C Isotropic = 58.7909 Anisotropy = 119.6837
XX= 38.3386 YX= 0.0000 ZX= -22.4798
XY= 0.0000 YY= 138.5801 ZY= 0.0000
XZ= -35.4974 YZ= 0.0000 ZZ= -0.5459
Eigenvalues: -16.0083 53.8011 138.5801
9 C Isotropic = 75.6978 Anisotropy = 104.1259
XX= 63.6720 YX= 0.0000 ZX= -13.6471
XY= 0.0000 YY= 145.1151 ZY= 0.0000
XZ= -6.8837 YZ= 0.0000 ZZ= 18.3064
Eigenvalues: 16.0917 65.8867 145.1151
10 C Isotropic = 25.9683 Anisotropy = 75.9175
XX= -22.7734 YX= 0.0000 ZX= 33.3326
XY= 0.0000 YY= 76.5800 ZY= 0.0000
XZ= 41.3372 YZ= 0.0000 ZZ= 24.0984
Eigenvalues: -43.4185 44.7435 76.5800
11 Br Isotropic = 1897.9319 Anisotropy = 1569.5179
XX= 1563.3369 YX= 0.0000 ZX= 437.7084
XY= 0.0000 YY= 1329.6002 ZY= 0.0000
XZ= 452.3533 YZ= 0.0000 ZZ= 2800.8586
Eigenvalues: 1329.6002 1419.9184 2944.2772
12 O Isotropic = 26.5214 Anisotropy = 219.4280
XX= -22.6771 YX= 0.0000 ZX= 4.7565

XY= 0.0000 YY= 172.8067 ZY= 0.0000
XZ= 50.7424 YZ= 0.0000 ZZ= -70.5654
Eigenvalues: -83.2730 -9.9694 172.8067
13 C Isotropic = 39.0102 Anisotropy = 91.6624
XX= 28.3887 YX= 0.0000 ZX= 41.9746
XY= 0.0000 YY= 100.1185 ZY= 0.0000
XZ= 41.1940 YZ= 0.0000 ZZ= -11.4766
Eigenvalues: -37.6587 54.5707 100.1185
14 C Isotropic = 69.6193 Anisotropy = 49.4395
XX= 101.8103 YX= 0.0000 ZX= 5.4445
XY= 0.0000 YY= 88.6900 ZY= 0.0000
XZ= -21.5367 YZ= 0.0000 ZZ= 18.3575
Eigenvalues: 17.5888 88.6900 102.5789
15 N Isotropic = -20.8027 Anisotropy = 290.9513
XX= -84.8138 YX= 0.0000 ZX= 73.3791
XY= 0.0000 YY= 173.1648 ZY= 0.0000
XZ= 38.9648 YZ= 0.0000 ZZ= -150.7592
Eigenvalues: -182.9209 -52.6521 173.1648
16 C Isotropic = 62.5884 Anisotropy = 102.3626
XX= 38.1796 YX= 0.0000 ZX= 25.5240
XY= 0.0000 YY= 130.8301 ZY= 0.0000
XZ= 30.3294 YZ= 0.0000 ZZ= 18.7554
Eigenvalues: -1.0998 58.0348 130.8301
17 N Isotropic = 95.9750 Anisotropy = 129.2082
XX= 72.2213 YX= 0.0000 ZX= -30.2626
XY= 0.0000 YY= 182.1138 ZY= 0.0000
XZ= -36.1118 YZ= 0.0000 ZZ= 33.5898
Eigenvalues: 14.5065 91.3046 182.1138
18 C Isotropic = 64.8977 Anisotropy = 114.8865
XX= 20.1493 YX= 0.0000 ZX= 44.3491
XY= 0.0000 YY= 141.4887 ZY= 0.0000
XZ= 32.4672 YZ= 0.0000 ZZ= 33.0551
Eigenvalues: -12.3442 65.5486 141.4887
19 C Isotropic = 72.6442 Anisotropy = 137.0756
XX= -5.8839 YX= 0.0000 ZX= -5.7973
XY= 0.0000 YY= 164.0279 ZY= 0.0000
XZ= -3.4546 YZ= 0.0000 ZZ= 59.7886
Eigenvalues: -6.2081 60.1129 164.0279
20 C Isotropic = 73.6037 Anisotropy = 130.8983
XX= 57.9694 YX= 0.0000 ZX= -7.6927
XY= 0.0000 YY= 160.8692 ZY= 0.0000
XZ= -5.6468 YZ= 0.0000 ZZ= 1.9724
Eigenvalues: 1.1890 58.7529 160.8692
21 I Isotropic = 3779.7198 Anisotropy = 1902.5835
XX= 3058.1925 YX= 0.0000 ZX= 519.7144
XY= 0.0000 YY= 3384.8181 ZY= 0.0000
XZ= 580.0815 YZ= 0.0000 ZZ= 4896.1488
Eigenvalues: 2906.2325 3384.8181 5048.1088
22 H Isotropic = 24.0366 Anisotropy = 10.5565
XX= 23.5676 YX= 0.0000 ZX= -1.7884
XY= 0.0000 YY= 17.9573 ZY= 0.0000
XZ= -2.0446 YZ= 0.0000 ZZ= 30.5850
Eigenvalues: 17.9573 23.0783 31.0743
23 H Isotropic = 24.1475 Anisotropy = 10.1383
XX= 28.0898 YX= 0.0000 ZX= 3.1310
XY= 0.0000 YY= 17.7093 ZY= 0.0000
XZ= 3.7993 YZ= 0.0000 ZZ= 26.6433
Eigenvalues: 17.7093 23.8267 30.9063

24 H Isotropic = 23.0940 Anisotropy = 10.5054
XX= 24.6605 YX= 0.0000 ZX= 2.0119
XY= 0.0000 YY= 15.4885 ZY= 0.0000
XZ= 2.5683 YZ= 0.0000 ZZ= 29.1330
Eigenvalues: 15.4885 23.6959 30.0976
25 H Isotropic = 23.9281 Anisotropy = 9.3054
XX= 28.7064 YX= 0.0000 ZX= -2.2694
XY= 0.0000 YY= 15.7468 ZY= 0.0000
XZ= -1.7265 YZ= 0.0000 ZZ= 27.3310
Eigenvalues: 15.7468 25.9057 30.1317
26 H Isotropic = 23.6582 Anisotropy = 6.2325
XX= 25.6911 YX= 0.0000 ZX= -0.3667
XY= 0.0000 YY= 18.1710 ZY= 0.0000
XZ= -2.0719 YZ= 0.0000 ZZ= 27.1127
Eigenvalues: 18.1710 24.9905 27.8132
27 H Isotropic = 22.1931 Anisotropy = 17.7814
XX= 33.7701 YX= 0.0000 ZX= 1.2853
XY= 0.0000 YY= 10.0653 ZY= 0.0000
XZ= 2.2548 YZ= 0.0000 ZZ= 22.7438
Eigenvalues: 10.0653 22.4666 34.0473
28 H Isotropic = 24.5923 Anisotropy = 4.0027
XX= 27.1233 YX= 0.0000 ZX= 0.1434
XY= 0.0000 YY= 20.8000 ZY= 0.0000
XZ= -1.0231 YZ= 0.0000 ZZ= 25.8537
Eigenvalues: 20.8000 25.7162 27.2608
29 H Isotropic = 25.1236 Anisotropy = 2.6554
XX= 26.8623 YX= 0.0000 ZX= 0.0888
XY= 0.0000 YY= 22.0873 ZY= 0.0000
XZ= -0.3332 YZ= 0.0000 ZZ= 26.4212
Eigenvalues: 22.0873 26.3896 26.8938
30 H Isotropic = 24.4931 Anisotropy = 5.6782
XX= 28.1753 YX= 0.0000 ZX= -0.7190
XY= 0.0000 YY= 19.4069 ZY= 0.0000
XZ= -0.2729 YZ= 0.0000 ZZ= 25.8971
Eigenvalues: 19.4069 25.7938 28.2786

Isomer 2 (conformer 4)

1 C Isotropic = 56.5703 Anisotropy = 145.8179
XX= -37.2714 YX= 0.2941 ZX= -23.0050
XY= -0.0122 YY= 153.7672 ZY= -1.1688
XZ= -19.1640 YZ= -1.2211 ZZ= 53.2151
Eigenvalues: -41.9432 57.8719 153.7822
2 C Isotropic = 46.8110 Anisotropy = 113.5066
XX= 57.7378 YX= 0.0410 ZX= -14.5036
XY= 0.0346 YY= 122.4551 ZY= -2.0946
XZ= -18.5974 YZ= -2.0161 ZZ= -39.7599
Eigenvalues: -42.5175 60.4685 122.4821
3 C Isotropic = 70.2731 Anisotropy = 125.3355
XX= 33.8913 YX= 1.0052 ZX= 39.5115
XY= 1.1936 YY= 153.8013 ZY= -1.9234
XZ= 34.6892 YZ= -1.7440 ZZ= 23.1267
Eigenvalues: -9.0070 65.9962 153.8301
4 C Isotropic = 46.3362 Anisotropy = 138.6360
XX= -27.8571 YX= 0.6466 ZX= -14.3980
XY= 0.6675 YY= 138.7413 ZY= -1.2789
XZ= -13.7476 YZ= -1.2732 ZZ= 28.1243
Eigenvalues: -31.1964 31.4447 138.7601
5 C Isotropic = 59.2016 Anisotropy = 164.3116
XX= 21.5204 YX= 0.6823 ZX= 0.2286
XY= 0.6473 YY= 168.7170 ZY= -1.9779
XZ= 0.0561 YZ= -2.0709 ZZ= -12.6328
Eigenvalues: -12.6561 21.5181 168.7426
6 C Isotropic = 58.0665 Anisotropy = 177.1955
XX= -18.0739 YX= 1.2014 ZX= 30.5013
XY= 1.4137 YY= 176.1708 ZY= -1.5358
XZ= 34.8086 YZ= -2.1673 ZZ= 16.1027
Eigenvalues: -37.8617 35.8644 176.1968
7 N Isotropic = 114.7861 Anisotropy = 86.0056
XX= 57.9742 YX= 0.8380 ZX= 32.6743
XY= 0.7565 YY= 172.1055 ZY= -1.2388
XZ= 20.9177 YZ= -0.7127 ZZ= 114.2787
Eigenvalues: 47.2506 124.9846 172.1232
8 C Isotropic = 61.3638 Anisotropy = 116.2921
XX= 46.4832 YX= 0.2879 ZX= -15.2020
XY= 0.4694 YY= 138.8764 ZY= -1.2623
XZ= -32.3063 YZ= -1.2737 ZZ= -1.2682
Eigenvalues: -11.0791 56.2786 138.8918
9 C Isotropic = 75.2521 Anisotropy = 106.3870
XX= 63.7502 YX= 0.3116 ZX= -9.4340
XY= 0.1609 YY= 146.1635 ZY= -1.1709
XZ= -1.2833 YZ= -1.3586 ZZ= 15.8426
Eigenvalues: 15.2390 64.3406 146.1768
10 C Isotropic = 26.7136 Anisotropy = 78.2967
XX= 38.7999 YX= 1.4092 ZX= -17.8998
XY= 3.2387 YY= 78.7609 ZY= -0.9748
XZ= -25.5205 YZ= 0.9124 ZZ= -37.4199
Eigenvalues: -43.1726 44.4021 78.9114
11 Br Isotropic = 1891.3090 Anisotropy = 1577.6786
XX= 1495.5547 YX= 3.7156 ZX= 313.3027
XY= 1.8255 YY= 1307.7893 ZY= 16.1650
XZ= 333.7163 YZ= 19.7449 ZZ= 2870.5828
Eigenvalues: 1307.5757 1423.2565 2943.0947
12 O Isotropic = 31.3650 Anisotropy = 203.9727
XX= -15.5139 YX= 4.9508 ZX= 59.8019

XY= 6.5370 YY= 167.1662 ZY= -2.7093
XZ= 4.0434 YZ= 1.0570 ZZ= -57.5573
Eigenvalues: -74.8075 1.5558 167.3468
13 C Isotropic = 39.4145 Anisotropy = 91.2474
XX= 49.8427 YX= 1.8128 ZX= 21.9212
XY= 1.5258 YY= 100.1896 ZY= -0.1912
XZ= 23.7831 YZ= -0.5490 ZZ= -31.7888
Eigenvalues: -37.7551 55.7525 100.2462
14 C Isotropic = 69.3162 Anisotropy = 50.1631
XX= 50.2817 YX= 1.6654 ZX= 28.4224
XY= 2.1742 YY= 87.8089 ZY= 1.3536
XZ= 54.5663 YZ= -2.0784 ZZ= 69.8579
Eigenvalues: 17.3941 87.7962 102.7582
15 N Isotropic = -25.0730 Anisotropy = 300.9107
XX= -79.9443 YX= 7.3709 ZX= 31.6924
XY= 8.9289 YY= 175.2738 ZY= -0.4633
XZ= 50.6654 YZ= -1.4628 ZZ= -170.5484
Eigenvalues: -186.5078 -64.2452 175.5341
16 C Isotropic = 62.8866 Anisotropy = 102.9316
XX= 55.9490 YX= -2.7309 ZX= 13.5677
XY= -2.1665 YY= 131.3274 ZY= 3.8733
XZ= 9.1213 YZ= 4.0642 ZZ= 1.3835
Eigenvalues: -1.0255 58.1777 131.5077
17 N Isotropic = 96.7317 Anisotropy = 128.4214
XX= 18.7849 YX= -5.4233 ZX= 14.7529
XY= -5.2260 YY= 182.1574 ZY= 0.7972
XZ= 20.9332 YZ= 2.7260 ZZ= 89.2529
Eigenvalues: 14.3384 93.5108 182.3460
18 C Isotropic = 64.4715 Anisotropy = 114.9133
XX= 64.8104 YX= -1.8664 ZX= -10.7610
XY= -2.9762 YY= 140.8323 ZY= 5.4547
XZ= 1.4831 YZ= 4.4869 ZZ= -12.2283
Eigenvalues: -12.6579 64.9919 141.0803
19 C Isotropic = 72.2926 Anisotropy = 136.4000
XX= 24.4349 YX= -2.7597 ZX= -31.1350
XY= -3.1187 YY= 163.0498 ZY= 3.1401
XZ= -34.1751 YZ= 3.0556 ZZ= 29.3930
Eigenvalues: -5.8350 59.4869 163.2259
20 C Isotropic = 74.2784 Anisotropy = 132.3582
XX= 23.4268 YX= -4.5372 ZX= 28.4596
XY= -4.8963 YY= 162.2890 ZY= 3.0947
XZ= 25.6655 YZ= 4.4634 ZZ= 37.1192
Eigenvalues: 2.1299 58.1881 162.5171
21 I Isotropic = 3738.1896 Anisotropy = 1951.9011
XX= 4536.4800 YX= -32.7116 ZX= -885.2203
XY= -75.2940 YY= 3294.8390 ZY= 33.3670
XZ= -934.2862 YZ= 44.1179 ZZ= 3383.2500
Eigenvalues: 2882.6162 3292.4957 5039.4570
22 H Isotropic = 24.0416 Anisotropy = 10.4539
XX= 24.0073 YX= -0.0671 ZX= -2.3998
XY= -0.0291 YY= 18.0046 ZY= 0.1884
XZ= -2.6076 YZ= 0.1524 ZZ= 30.1131
Eigenvalues: 18.0021 23.1119 31.0109
23 H Isotropic = 24.2399 Anisotropy = 10.0223
XX= 27.5308 YX= -0.0046 ZX= 3.1281
XY= 0.0245 YY= 17.8470 ZY= 0.0840
XZ= 3.8388 YZ= 0.1005 ZZ= 27.3420
Eigenvalues: 17.8460 23.9523 30.9215

24 H Isotropic = 22.9167 Anisotropy = 10.4991
XX= 23.7273 YX= -0.0504 ZX= 1.6531
XY= -0.0283 YY= 15.6861 ZY= 0.2299
XZ= 2.1264 YZ= 0.1615 ZZ= 29.3367
Eigenvalues: 15.6827 23.1513 29.9161
25 H Isotropic = 24.0071 Anisotropy = 9.4455
XX= 29.1878 YX= -0.0885 ZX= -2.1992
XY= -0.0778 YY= 15.7913 ZY= 0.0956
XZ= -1.6146 YZ= 0.1179 ZZ= 27.0422
Eigenvalues: 15.7900 25.9273 30.3041
26 H Isotropic = 23.9177 Anisotropy = 6.2250
XX= 26.4662 YX= -0.0443 ZX= -0.3138
XY= -0.0146 YY= 18.2010 ZY= 0.0951
XZ= -2.1927 YZ= 0.0679 ZZ= 27.0858
Eigenvalues: 18.2002 25.4851 28.0677
27 H Isotropic = 22.2261 Anisotropy = 17.6690
XX= 29.4123 YX= -0.3598 ZX= 6.3527
XY= 0.0531 YY= 10.6539 ZY= -0.9361
XZ= 5.2626 YZ= -0.8387 ZZ= 26.6123
Eigenvalues: 10.6030 22.0699 34.0055
28 H Isotropic = 24.7331 Anisotropy = 4.0082
XX= 26.1394 YX= 0.0786 ZX= 0.0051
XY= -0.0349 YY= 20.9955 ZY= -0.1529
XZ= 1.3024 YZ= -0.1531 ZZ= 27.0645
Eigenvalues: 20.9913 25.8028 27.4053
29 H Isotropic = 25.2076 Anisotropy = 2.6861
XX= 26.5323 YX= 0.0559 ZX= 0.1282
XY= 0.0294 YY= 22.3753 ZY= -0.1028
XZ= 0.5971 YZ= -0.0985 ZZ= 26.7150
Eigenvalues: 22.3723 26.2521 26.9983
30 H Isotropic = 24.7678 Anisotropy = 5.7414
XX= 26.7734 YX= 0.0698 ZX= 1.7328
XY= 0.2198 YY= 20.1852 ZY= 0.0202
XZ= 1.2851 YZ= -0.0823 ZZ= 27.3448
Eigenvalues: 20.1814 25.5266 28.5954

Isomer 3 (conformer 1)

1 C Isotropic = 58.3732 Anisotropy = 142.7849
XX= 2.8113 YX= 35.6547 ZX= 43.8245
XY= 38.2708 YY= 39.7773 ZY= -41.5848
XZ= 42.9336 YZ= -39.5323 ZZ= 132.5310
Eigenvalues: -39.8508 61.4073 153.5631
2 C Isotropic = 47.5605 Anisotropy = 111.0675
XX= -7.3379 YX= -49.4208 ZX= 13.8003
XY= -51.8803 YY= 35.1272 ZY= -13.8809
XZ= 11.5031 YZ= -14.3549 ZZ= 114.8921
Eigenvalues: -41.0745 62.1504 121.6055
3 C Isotropic = 70.8149 Anisotropy = 123.0722
XX= 69.9350 YX= -13.5147 ZX= 14.4985
XY= -17.8368 YY= 4.8608 ZY= -39.6495
XZ= 12.7420 YZ= -41.9697 ZZ= 137.6489
Eigenvalues: -8.3732 67.9548 152.8631
4 C Isotropic = 47.0363 Anisotropy = 141.4355
XX= -2.8981 YX= 17.4428 ZX= 37.4795
XY= 18.0988 YY= 22.3656 ZY= -39.3974
XZ= 37.3849 YZ= -38.0683 ZZ= 121.6414
Eigenvalues: -29.8277 29.6100 141.3267
5 C Isotropic = 56.6692 Anisotropy = 165.0984
XX= 8.7345 YX= -21.1826 ZX= 28.8425
XY= -23.7027 YY= 12.4976 ZY= -39.1171
XZ= 29.3803 YZ= -39.8498 ZZ= 148.7753
Eigenvalues: -12.1644 15.4371 166.7348
6 C Isotropic = 58.8983 Anisotropy = 172.5117
XX= 45.9074 YX= 0.8005 ZX= 28.9864
XY= 1.5363 YY= -19.1932 ZY= -56.2600
XZ= 35.7749 YZ= -54.5684 ZZ= 149.9805
Eigenvalues: -37.1025 39.8912 173.9061
7 N Isotropic = 116.5993 Anisotropy = 83.6093
XX= 122.8495 YX= 21.6417 ZX= 16.2535
XY= 16.6330 YY= 66.4187 ZY= -34.4097
XZ= 11.3615 YZ= -32.2654 ZZ= 160.5298
Eigenvalues: 48.9599 128.4993 172.3389
8 C Isotropic = 60.8396 Anisotropy = 117.6032
XX= 0.0533 YX= -26.9016 ZX= 22.4281
XY= -31.0744 YY= 54.6820 ZY= -18.5605
XZ= 19.0409 YZ= -24.0747 ZZ= 127.7834
Eigenvalues: -13.3140 56.5910 139.2417
9 C Isotropic = 74.1015 Anisotropy = 112.6218
XX= 37.2711 YX= -33.7324 ZX= 14.6443
XY= -26.7984 YY= 46.1312 ZY= -23.8378
XZ= 18.4599 YZ= -21.7269 ZZ= 138.9021
Eigenvalues: 11.0642 62.0575 149.1827
10 Br Isotropic = 1892.3011 Anisotropy = 1566.3861
XX= 2537.7418 YX= 654.1385 ZX= -74.1187
XY= 679.1287 YY= 1808.2287 ZY= -5.9323
XZ= -87.6843 YZ= -22.2770 ZZ= 1330.9328
Eigenvalues: 1318.3326 1422.0121 2936.5585
11 C Isotropic = 38.6289 Anisotropy = 105.6737
XX= 70.4835 YX= -10.1932 ZX= 30.0554
XY= -13.0041 YY= -9.1752 ZY= -53.2161
XZ= 22.3528 YZ= -60.8477 ZZ= 54.5783
Eigenvalues: -42.7333 49.5419 109.0780
12 C Isotropic = 65.9702 Anisotropy = 85.6317
XX= 77.8930 YX= 46.3850 ZX= 25.4265

XY= 39.3475 YY= 80.9055 ZY= -32.0540
XZ= 33.0256 YZ= -3.8812 ZZ= 39.1122
Eigenvalues: 4.0566 70.7960 123.0580
13 O Isotropic = 22.3935 Anisotropy = 187.0886
XX= 55.7803 YX= -72.5078 ZX= 35.0765
XY= -49.9654 YY= -49.2379 ZY= -72.2334
XZ= 67.3491 YZ= -48.5308 ZZ= 60.6380
Eigenvalues: -86.9319 6.9932 147.1192
14 C Isotropic = 22.7256 Anisotropy = 84.7024
XX= 28.4138 YX= -2.2762 ZX= 42.8033
XY= 7.4098 YY= 23.7901 ZY= -39.3926
XZ= 51.7163 YZ= -30.6025 ZZ= 15.9730
Eigenvalues: -38.8694 27.8524 79.1939
15 N Isotropic = -6.9714 Anisotropy = 322.8780
XX= 46.6387 YX= -43.4631 ZX= 111.3168
XY= -61.2755 YY= -101.2071 ZY= -123.3713
XZ= 113.3313 YZ= -139.9989 ZZ= 33.6543
Eigenvalues: -182.8071 -46.3876 208.2806
16 I Isotropic = 3694.8078 Anisotropy = 2074.4287
XX= 3808.2998 YX= -454.3049 ZX= -752.7268
XY= -360.2641 YY= 2937.4880 ZY= 210.9434
XZ= -1020.4052 YZ= 202.1779 ZZ= 4338.6356
Eigenvalues: 2757.1750 3249.4881 5077.7603
17 N Isotropic = 97.9892 Anisotropy = 124.3770
XX= 82.8032 YX= -62.5556 ZX= 49.9329
XY= -59.5336 YY= 78.7897 ZY= -6.3493
XZ= 52.5084 YZ= -4.6723 ZZ= 132.3747
Eigenvalues: 10.5452 102.5152 180.9072
18 C Isotropic = 62.3929 Anisotropy = 99.8389
XX= 66.0041 YX= -3.2619 ZX= 53.4768
XY= -8.8064 YY= 57.9650 ZY= -33.1662
XZ= 49.9903 YZ= -37.7927 ZZ= 63.2095
Eigenvalues: 3.3135 54.9129 128.9521
19 C Isotropic = 70.7724 Anisotropy = 142.0082
XX= 57.3829 YX= -37.1846 ZX= 72.8438
XY= -34.7303 YY= 66.3591 ZY= -26.3649
XZ= 73.1840 YZ= -23.0029 ZZ= 88.5752
Eigenvalues: -4.2945 51.1672 165.4446
20 C Isotropic = 71.2678 Anisotropy = 135.7057
XX= 92.6960 YX= -35.7270 ZX= 39.7303
XY= -36.3591 YY= 21.1297 ZY= -48.5015
XZ= 38.9528 YZ= -48.8666 ZZ= 99.9775
Eigenvalues: -5.2235 57.2886 161.7382
21 C Isotropic = 62.9539 Anisotropy = 118.6729
XX= 79.2876 YX= -4.1070 ZX= 52.3866
XY= 0.7198 YY= 45.2445 ZY= -55.6954
XZ= 55.8071 YZ= -51.1557 ZZ= 64.3294
Eigenvalues: -13.7570 60.5495 142.0691
22 H Isotropic = 24.1708 Anisotropy = 10.2069
XX= 25.0127 YX= 3.8794 ZX= -0.5840
XY= 3.1957 YY= 28.5177 ZY= 2.3909
XZ= -0.4525 YZ= 2.3660 ZZ= 18.9821
Eigenvalues: 18.1272 23.4099 30.9754
23 H Isotropic = 24.1232 Anisotropy = 10.3471
XX= 30.3190 YX= 0.1046 ZX= -3.0304
XY= 0.5203 YY= 23.3793 ZY= 1.6303
XZ= -2.8533 YZ= 1.8767 ZZ= 18.6713
Eigenvalues: 17.4382 23.9101 31.0213

 24 H Isotropic = 23.1374 Anisotropy = 10.7739
XX= 29.1409 YX= 3.0739 ZX= -2.4175
XY= 2.6611 YY= 22.6694 ZY= 2.0869
XZ= -1.6661 YZ= 2.8576 ZZ= 17.6019
Eigenvalues: 15.9043 23.1879 30.3200
 25 H Isotropic = 23.9271 Anisotropy = 9.4200
XX= 25.3467 YX= -0.1492 ZX= -2.7072
XY= 0.7056 YY= 29.1164 ZY= 3.6288
XZ= -2.4291 YZ= 3.7062 ZZ= 17.3181
Eigenvalues: 15.6048 25.9693 30.2071
 26 H Isotropic = 23.8210 Anisotropy = 11.0560
XX= 23.8110 YX= 4.0799 ZX= -2.6087
XY= 1.9722 YY= 29.8992 ZY= 0.8268
XZ= -1.8988 YZ= -0.6036 ZZ= 17.7528
Eigenvalues: 16.9127 23.3587 31.1917
 27 H Isotropic = 22.8366 Anisotropy = 8.2844
XX= 22.5823 YX= 3.9187 ZX= -4.0173
XY= 3.8743 YY= 25.6545 ZY= 2.9747
XZ= -4.0222 YZ= 3.7240 ZZ= 20.2729
Eigenvalues: 14.8817 25.2684 28.3595
 28 H Isotropic = 24.4751 Anisotropy = 5.9650
XX= 23.1115 YX= 1.1163 ZX= -1.5331
XY= 0.9425 YY= 26.9010 ZY= 2.8866
XZ= -1.7758 YZ= 2.6993 ZZ= 23.4127
Eigenvalues: 20.4437 24.5298 28.4517
 29 H Isotropic = 25.1869 Anisotropy = 2.6727
XX= 24.9571 YX= 0.6381 ZX= -1.7985
XY= 0.9627 YY= 26.0577 ZY= 1.2830
XZ= -1.5339 YZ= 1.6150 ZZ= 24.5458
Eigenvalues: 22.3604 26.2315 26.9687
 30 H Isotropic = 24.6724 Anisotropy = 3.4245
XX= 24.3512 YX= 0.5060 ZX= -2.3425
XY= 1.4123 YY= 25.6371 ZY= 1.3801
XZ= -1.9366 YZ= 2.3200 ZZ= 24.0290
Eigenvalues: 21.1362 25.9257 26.9555

Isomer 3 (conformer 2)

```
  1  C    Isotropic =    59.0721   Anisotropy =   142.9679
XX=    24.6506   YX=    43.9568   ZX=    13.3187
XY=    47.9028   YY=    11.7131   ZY=   -45.2399
XZ=    13.7719   YZ=   -42.6258   ZZ=   140.8526
Eigenvalues:   -38.2601    61.0924   154.3840
  2  C    Isotropic =    47.7737   Anisotropy =   111.2550
XX=   -33.1325   YX=   -23.6539   ZX=    -7.6848
XY=   -24.7349   YY=    61.3309   ZY=   -19.6897
XZ=   -13.4649   YZ=   -20.8498   ZZ=   115.1228
Eigenvalues:   -40.4476    61.8251   121.9437
  3  C    Isotropic =    70.2546   Anisotropy =   124.2649
XX=    53.5240   YX=   -24.2132   ZX=    -8.3946
XY=   -29.1462   YY=    20.3261   ZY=   -45.5495
XZ=   -10.3329   YZ=   -47.1609   ZZ=   136.9136
Eigenvalues:    -8.7055    66.3714   153.0979
  4  C    Isotropic =    47.3786   Anisotropy =   141.6666
XX=     8.0682   YX=    26.6687   ZX=    10.7566
XY=    28.7784   YY=     9.3212   ZY=   -48.1358
XZ=     8.1369   YZ=   -46.9940   ZZ=   124.7463
Eigenvalues:   -30.1779    30.4906   141.8229
  5  C    Isotropic =    58.1336   Anisotropy =   164.9929
XX=    -4.8625   YX=    -8.2683   ZX=    -3.4413
XY=   -11.1476   YY=    26.6263   ZY=   -45.7520
XZ=    -1.8989   YZ=   -47.8836   ZZ=   152.6369
Eigenvalues:    -9.7135    15.9854   168.1288
  6  C    Isotropic =    59.2506   Anisotropy =   173.0274
XX=    38.9256   YX=    -8.9035   ZX=    -1.9351
XY=    -9.3807   YY=   -16.7593   ZY=   -58.6673
XZ=     5.5229   YZ=   -61.4709   ZZ=   155.5854
Eigenvalues:   -36.5185    39.6681   174.6022
  7  N    Isotropic =   115.8934   Anisotropy =    86.1885
XX=   127.6417   YX=     7.2241   ZX=     2.5419
XY=     0.8494   YY=    60.2476   ZY=   -39.5600
XZ=    -3.6714   YZ=   -38.5257   ZZ=   159.7910
Eigenvalues:    46.5986   127.7293   173.3524
  8  C    Isotropic =    60.3994   Anisotropy =   115.0133
XX=   -16.6248   YX=     1.5107   ZX=     1.7690
XY=   -10.0212   YY=    68.7069   ZY=   -22.8704
XZ=     0.6835   YZ=   -23.6461   ZZ=   129.1160
Eigenvalues:   -16.8365    60.9597   137.0749
  9  C    Isotropic =    73.3397   Anisotropy =   112.7402
XX=    14.2664   YX=   -23.3326   ZX=    -5.9254
XY=   -18.2513   YY=    65.2285   ZY=   -27.8682
XZ=    -3.8845   YZ=   -23.6153   ZZ=   140.5243
Eigenvalues:     5.4805    66.0389   148.4999
 10  Br   Isotropic =  1902.8070   Anisotropy =  1576.1315
XX=  2884.6164   YX=   292.9046   ZX=    96.6274
XY=   307.5245   YY=  1475.0676   ZY=    50.8292
XZ=   106.7773   YZ=    61.6923   ZZ=  1348.7371
Eigenvalues:  1327.1705  1427.6893  2953.5613
 11  C    Isotropic =    38.8285   Anisotropy =   105.0445
XX=    11.9508   YX=   -65.4953   ZX=    29.0618
XY=   -67.7319   YY=    41.5670   ZY=   -11.7280
XZ=    31.1657   YZ=    -2.9255   ZZ=    62.9678
Eigenvalues:   -44.9314    52.5588   108.8582
 12  C    Isotropic =    60.7278   Anisotropy =    77.1436
XX=    41.8446   YX=     0.4736   ZX=    52.0830
```

XY= 0.6488 YY= 92.5648 ZY= 27.5768
XZ= 42.0511 YZ= 22.4249 ZZ= 47.7740
Eigenvalues: -5.3096 75.3361 112.1569
13 O Isotropic = 16.6824 Anisotropy = 190.2427
XX= 3.1118 YX= -97.5193 ZX= 39.9596
XY= -104.8483 YY= 24.3867 ZY= -31.8873
XZ= 12.5734 YZ= -76.7001 ZZ= 22.5486
Eigenvalues: -90.8993 -2.5645 143.5109
14 C Isotropic = 22.6608 Anisotropy = 86.4855
XX= 13.5854 YX= -23.7186 ZX= 50.4931
XY= -28.2769 YY= 50.9514 ZY= -4.1206
XZ= 42.5845 YZ= -18.0812 ZZ= 3.4457
Eigenvalues: -39.2992 26.9639 80.3178
15 N Isotropic = -12.8548 Anisotropy = 310.4865
XX= -43.3478 YX= -149.2374 ZX= 82.2260
XY= -156.3473 YY= 12.9898 ZY= -60.8227
XZ= 111.9576 YZ= -46.4007 ZZ= -8.2063
Eigenvalues: -182.0943 -50.6062 194.1362
16 I Isotropic = 3701.6263 Anisotropy = 2065.9302
XX= 3618.8424 YX= -211.4629 ZX= -933.4304
XY= -231.2537 YY= 2960.7031 ZY= -120.4529
XZ= -864.3217 YZ= -111.5821 ZZ= 4525.3333
Eigenvalues: 2758.2178 3267.7480 5078.9131
17 N Isotropic = 98.1072 Anisotropy = 124.9296
XX= 127.7148 YX= -39.5591 ZX= 10.5307
XY= -43.5155 YY= 96.4986 ZY= -67.0027
XZ= 9.1758 YZ= -69.7379 ZZ= 70.1080
Eigenvalues: 10.3550 102.5729 181.3935
18 C Isotropic = 62.4760 Anisotropy = 100.6553
XX= 56.2788 YX= -34.6768 ZX= 42.7940
XY= -30.2126 YY= 87.5330 ZY= -22.2446
XZ= 48.0895 YZ= -17.5286 ZZ= 43.6161
Eigenvalues: 3.4899 54.3585 129.5795
19 C Isotropic = 71.2512 Anisotropy = 142.3407
XX= 86.6617 YX= -38.1287 ZX= 44.8613
XY= -38.5940 YY= 93.7200 ZY= -55.0821
XZ= 41.1246 YZ= -57.0952 ZZ= 33.3718
Eigenvalues: -4.4958 52.1043 166.1450
20 C Isotropic = 71.6906 Anisotropy = 135.3089
XX= 59.8601 YX= -72.0171 ZX= 24.8691
XY= -71.3419 YY= 74.3894 ZY= -35.7447
XZ= 24.6538 YZ= -35.0861 ZZ= 80.8224
Eigenvalues: -5.3156 58.4909 161.8966
21 C Isotropic = 63.2693 Anisotropy = 118.2511
XX= 44.0767 YX= -45.9720 ZX= 56.6592
XY= -49.7335 YY= 91.0761 ZY= -10.8164
XZ= 51.9124 YZ= -15.8755 ZZ= 54.6552
Eigenvalues: -13.0493 60.7538 142.1034
22 H Isotropic = 24.1598 Anisotropy = 10.5783
XX= 27.6775 YX= 3.8954 ZX= 1.9187
XY= 3.0934 YY= 25.5810 ZY= 2.7571
XZ= 2.2500 YZ= 2.8006 ZZ= 19.2210
Eigenvalues: 18.1098 23.1576 31.2121
23 H Isotropic = 24.1196 Anisotropy = 9.7883
XX= 29.8304 YX= -2.3056 ZX= -0.7285
XY= -1.8202 YY= 23.9566 ZY= 2.4360
XZ= -0.6173 YZ= 2.3721 ZZ= 18.5717
Eigenvalues: 17.6537 24.0600 30.6451

24 H Isotropic = 23.6836 Anisotropy = 11.1711
XX= 29.6806 YX= -0.3248 ZX= 3.1835
XY= -1.2345 YY= 20.2851 ZY= 1.8050
XZ= 4.4480 YZ= 1.7435 ZZ= 21.0850
Eigenvalues: 17.9974 21.9223 31.1310
25 H Isotropic = 24.1467 Anisotropy = 10.1893
XX= 25.5563 YX= -0.0599 ZX= -0.3114
XY= 0.8202 YY= 28.8621 ZY= 4.9962
XZ= -0.2242 YZ= 5.3300 ZZ= 18.0216
Eigenvalues: 15.9403 25.5602 30.9396
26 H Isotropic = 24.2429 Anisotropy = 6.0820
XX= 24.9341 YX= 0.8644 ZX= -0.5841
XY= 0.0362 YY= 27.2540 ZY= 3.4660
XZ= -0.5652 YZ= 2.1763 ZZ= 20.5407
Eigenvalues: 19.4251 25.0061 28.2976
27 H Isotropic = 22.9797 Anisotropy = 7.4174
XX= 22.7711 YX= 4.7297 ZX= -2.1243
XY= 4.8497 YY= 22.5852 ZY= 4.0662
XZ= -2.8062 YZ= 3.8678 ZZ= 23.5829
Eigenvalues: 15.3403 25.6742 27.9247
28 H Isotropic = 24.4874 Anisotropy = 6.0355
XX= 25.8340 YX= 3.2476 ZX= -1.6589
XY= 3.3722 YY= 24.1295 ZY= 0.7229
XZ= -1.4978 YZ= 1.0068 ZZ= 23.4987
Eigenvalues: 20.6017 24.3495 28.5111
29 H Isotropic = 25.1641 Anisotropy = 2.6135
XX= 25.4774 YX= 1.7801 ZX= -1.0657
XY= 1.4967 YY= 24.7295 ZY= 1.2983
XZ= -1.4638 YZ= 0.8279 ZZ= 25.2853
Eigenvalues: 22.4796 26.1062 26.9064
30 H Isotropic = 24.7270 Anisotropy = 3.4468
XX= 25.0911 YX= 2.3099 ZX= -1.2489
XY= 1.7245 YY= 24.0202 ZY= 1.6654
XZ= -2.2533 YZ= 0.8342 ZZ= 25.0696
Eigenvalues: 21.3171 25.8390 27.0248

Isomer 3 (conformer 3)

1 C Isotropic = 58.3684 Anisotropy = 142.8612
XX= 12.4764 YX= 34.5919 ZX= 41.0526
XY= 37.2144 YY= 40.5251 ZY= -56.3690
XZ= 41.3439 YZ= -54.5894 ZZ= 122.1038
Eigenvalues: -39.2969 60.7929 153.6092
2 C Isotropic = 47.6339 Anisotropy = 110.9693
XX= -19.8615 YX= -43.0433 ZX= 7.3404
XY= -45.8771 YY= 51.6464 ZY= -22.1564
XZ= 4.2328 YZ= -22.1442 ZZ= 111.1168
Eigenvalues: -41.2886 62.5769 121.6134
3 C Isotropic = 70.7238 Anisotropy = 123.2343
XX= 64.6201 YX= -21.4129 ZX= 6.7291
XY= -25.6040 YY= 20.1247 ZY= -54.0052
XZ= 4.2745 YZ= -55.7818 ZZ= 127.4265
Eigenvalues: -8.3061 67.5974 152.8800
4 C Isotropic = 46.9822 Anisotropy = 141.8194
XX= 1.5962 YX= 17.3155 ZX= 33.5629
XY= 17.5753 YY= 27.5595 ZY= -53.8858
XZ= 33.3254 YZ= -53.0615 ZZ= 111.7908
Eigenvalues: -30.2354 29.6536 141.5284
5 C Isotropic = 57.0836 Anisotropy = 165.1024
XX= 2.6608 YX= -22.9195 ZX= 19.8019
XY= -25.3206 YY= 29.8058 ZY= -55.4059
XZ= 20.1025 YZ= -56.5901 ZZ= 138.7844
Eigenvalues: -12.7778 16.8769 167.1519
6 C Isotropic = 58.4380 Anisotropy = 174.3798
XX= 42.5296 YX= -9.4283 ZX= 20.3647
XY= -8.3368 YY= -3.2501 ZY= -76.2404
XZ= 27.0599 YZ= -76.7903 ZZ= 136.0346
Eigenvalues: -37.0990 37.7219 174.6912
7 N Isotropic = 117.0942 Anisotropy = 83.2537
XX= 127.6745 YX= 12.7341 ZX= 12.7472
XY= 8.3311 YY= 71.1633 ZY= -46.1323
XZ= 7.8920 YZ= -42.6043 ZZ= 152.4448
Eigenvalues: 49.2030 129.4829 172.5966
8 C Isotropic = 60.8920 Anisotropy = 117.7174
XX= -5.8547 YX= -19.5869 ZX= 16.8346
XY= -25.4277 YY= 66.3268 ZY= -28.3528
XZ= 12.1162 YZ= -33.3013 ZZ= 122.2039
Eigenvalues: -12.5406 55.8463 139.3703
9 C Isotropic = 73.9781 Anisotropy = 113.3115
XX= 28.4389 YX= -33.5953 ZX= 6.4361
XY= -25.9487 YY= 61.1950 ZY= -34.2294
XZ= 11.7002 YZ= -34.5169 ZZ= 132.3002
Eigenvalues: 9.9467 62.4684 149.5190
10 Br Isotropic = 1906.7642 Anisotropy = 1563.5366
XX= 2712.2820 YX= 540.2855 ZX= -21.6310
XY= 564.3236 YY= 1660.9153 ZY= 37.8992
XZ= -22.8861 YZ= 26.1766 ZZ= 1347.0952
Eigenvalues: 1331.3182 1439.8524 2949.1219
11 C Isotropic = 38.1763 Anisotropy = 106.1867
XX= 62.9529 YX= -22.0220 ZX= 19.7760
XY= -23.7423 YY= 5.6033 ZY= -63.2766
XZ= 12.5893 YZ= -65.8331 ZZ= 45.9728
Eigenvalues: -42.6295 48.1911 108.9674
12 C Isotropic = 69.6714 Anisotropy = 90.1715
XX= 91.5691 YX= 47.2430 ZX= 27.9209

XY= 37.3453 YY= 77.6163 ZY= -27.2083
XZ= 34.4029 YZ= -4.5549 ZZ= 39.8288
Eigenvalues: 7.7020 71.5265 129.7857
 13 O Isotropic = 27.3626 Anisotropy = 182.2416
XX= 36.6781 YX= -80.7682 ZX= 18.3807
XY= -65.0704 YY= -8.6287 ZY= -81.5924
XZ= 48.2620 YZ= -68.4646 ZZ= 54.0383
Eigenvalues: -78.4736 11.7044 148.8570
 14 C Isotropic = 22.7642 Anisotropy = 82.7851
XX= 25.5017 YX= -4.1181 ZX= 37.1417
XY= 3.9171 YY= 32.3217 ZY= -41.6155
XZ= 47.2648 YZ= -36.4526 ZZ= 10.4691
Eigenvalues: -38.6736 29.0119 77.9542
 15 N Isotropic = -14.1762 Anisotropy = 330.9499
XX= 21.0610 YX= -60.5131 ZX= 89.8142
XY= -86.1912 YY= -65.4858 ZY= -155.8096
XZ= 83.1522 YZ= -175.2160 ZZ= 1.8962
Eigenvalues: -200.7255 -48.2601 206.4571
 16 I Isotropic = 3699.9393 Anisotropy = 2105.7734
XX= 3759.4935 YX= -512.1786 ZX= -830.9952
XY= -394.4700 YY= 3033.9872 ZY= 195.7656
XZ= -1048.4998 YZ= 208.3960 ZZ= 4306.3372
Eigenvalues: 2755.6314 3240.3982 5103.7883
 17 N Isotropic = 99.0191 Anisotropy = 124.2753
XX= 57.8639 YX= -30.1122 ZX= 68.6342
XY= -30.6867 YY= 127.4230 ZY= -22.0317
XZ= 66.9653 YZ= -23.5223 ZZ= 111.7703
Eigenvalues: 10.4435 104.7445 181.8693
 18 C Isotropic = 61.6463 Anisotropy = 98.2467
XX= 59.4512 YX= -44.7293 ZX= 14.1687
XY= -40.3037 YY= 42.2148 ZY= -40.2721
XZ= 17.5794 YZ= -36.4867 ZZ= 83.2730
Eigenvalues: 1.6908 56.1041 127.1441
 19 C Isotropic = 70.1625 Anisotropy = 143.0213
XX= 40.9664 YX= -54.7361 ZX= 48.7815
XY= -55.8908 YY= 70.8242 ZY= -36.2955
XZ= 48.7542 YZ= -36.0734 ZZ= 98.6970
Eigenvalues: -5.1222 50.0997 165.5101
 20 C Isotropic = 70.7408 Anisotropy = 136.1889
XX= 76.1407 YX= -15.7715 ZX= 51.4088
XY= -15.7450 YY= 67.7474 ZY= -65.8651
XZ= 53.1474 YZ= -63.9869 ZZ= 68.3344
Eigenvalues: -6.8454 57.5345 161.5334
 21 C Isotropic = 63.6378 Anisotropy = 116.7187
XX= 74.8121 YX= -38.4249 ZX= 18.4517
XY= -41.9956 YY= 35.0911 ZY= -56.6001
XZ= 14.7043 YZ= -59.3830 ZZ= 81.0102
Eigenvalues: -11.7981 61.2612 141.4503
 22 H Isotropic = 24.1662 Anisotropy = 10.1752
XX= 25.9430 YX= 4.0719 ZX= 0.1547
XY= 3.5633 YY= 26.9597 ZY= 3.3793
XZ= 0.2323 YZ= 3.3238 ZZ= 19.5960
Eigenvalues: 18.0807 23.4683 30.9497
 23 H Isotropic = 24.1594 Anisotropy = 10.3435
XX= 30.3531 YX= -0.5442 ZX= -2.8518
XY= -0.1618 YY= 22.9057 ZY= 2.4173
XZ= -2.4277 YZ= 2.7301 ZZ= 19.2193
Eigenvalues: 17.5142 23.9089 31.0551

24 H Isotropic = 23.0386 Anisotropy = 10.4819
XX= 29.5032 YX= 2.2365 ZX= -1.8519
XY= 1.8050 YY= 21.5496 ZY= 2.8873
XZ= -1.0079 YZ= 3.4945 ZZ= 18.0629
Eigenvalues: 15.7937 23.2955 30.0265
25 H Isotropic = 23.9581 Anisotropy = 9.2195
XX= 25.5614 YX= 0.5587 ZX= -2.1012
XY= 1.3343 YY= 27.9394 ZY= 4.9795
XZ= -1.7373 YZ= 5.0915 ZZ= 18.3734
Eigenvalues: 15.7461 26.0237 30.1044
26 H Isotropic = 23.8701 Anisotropy = 11.2381
XX= 25.0652 YX= 5.4420 ZX= -1.8711
XY= 2.8099 YY= 28.6399 ZY= 2.2477
XZ= -1.5719 YZ= 0.9960 ZZ= 17.9052
Eigenvalues: 16.8993 23.3489 31.3622
27 H Isotropic = 23.0907 Anisotropy = 7.7985
XX= 24.0490 YX= 2.4478 ZX= -4.4595
XY= 2.4036 YY= 22.9465 ZY= 4.8037
XZ= -4.5100 YZ= 4.8100 ZZ= 22.2768
Eigenvalues: 15.0478 25.9347 28.2897
28 H Isotropic = 24.2151 Anisotropy = 5.5650
XX= 23.7268 YX= 0.9820 ZX= -1.7008
XY= 1.0789 YY= 24.7103 ZY= 3.0723
XZ= -1.4257 YZ= 3.7893 ZZ= 24.2083
Eigenvalues: 20.0809 24.6393 27.9251
29 H Isotropic = 25.0606 Anisotropy = 2.5089
XX= 25.1980 YX= 1.2183 ZX= -1.1129
XY= 0.9729 YY= 25.3777 ZY= 1.8091
XZ= -1.4419 YZ= 1.5768 ZZ= 24.6059
Eigenvalues: 22.2844 26.1641 26.7332
30 H Isotropic = 24.6698 Anisotropy = 3.6712
XX= 24.6929 YX= 1.8092 ZX= -1.0110
XY= 1.0989 YY= 25.2665 ZY= 2.6059
XZ= -1.7056 YZ= 2.0282 ZZ= 24.0501
Eigenvalues: 21.1646 25.7277 27.1173

Isomer 3 (conformer 4)

1 C Isotropic = 59.1885 Anisotropy = 142.5448
XX= 13.1217 YX= 45.6734 ZX= 15.0466
XY= 49.5948 YY= 17.0467 ZY= -31.6754
XZ= 14.0555 YZ= -28.9148 ZZ= 147.3971
Eigenvalues: -37.9747 61.3218 154.2184
2 C Isotropic = 48.1225 Anisotropy = 111.0331
XX= -25.4823 YX= -35.0139 ZX= -1.8692
XY= -36.7707 YY= 51.1070 ZY= -14.4861
XZ= -7.2545 YZ= -16.2407 ZZ= 118.7428
Eigenvalues: -40.2943 62.5173 122.1446
3 C Isotropic = 70.2648 Anisotropy = 124.6259
XX= 59.6340 YX= -19.2834 ZX= -0.4572
XY= -24.4880 YY= 6.6813 ZY= -34.4355
XZ= -1.3384 YZ= -36.8168 ZZ= 144.4792
Eigenvalues: -8.7422 66.1880 153.3487
4 C Isotropic = 47.2940 Anisotropy = 141.6302
XX= 1.0922 YX= 26.7269 ZX= 14.4110
XY= 28.4016 YY= 8.7577 ZY= -35.6398
XZ= 11.5866 YZ= -35.2348 ZZ= 132.0322
Eigenvalues: -29.8875 30.0555 141.7142
5 C Isotropic = 58.3564 Anisotropy = 165.5843
XX= -1.9531 YX= -11.5619 ZX= 3.9078
XY= -14.5565 YY= 16.3079 ZY= -33.2248
XZ= 6.3919 YZ= -35.0596 ZZ= 160.7145
Eigenvalues: -9.6685 15.9919 168.7459
6 C Isotropic = 59.7075 Anisotropy = 172.5697
XX= 41.0467 YX= -1.8151 ZX= 5.8444
XY= -1.0717 YY= -27.2541 ZY= -41.5229
XZ= 14.1213 YZ= -41.9997 ZZ= 165.3300
Eigenvalues: -35.9249 40.2935 174.7540
7 N Isotropic = 115.4158 Anisotropy = 87.3781
XX= 124.9826 YX= 16.1880 ZX= 6.1620
XY= 9.4499 YY= 54.9876 ZY= -29.5704
XZ= 0.0165 YZ= -29.6608 ZZ= 166.2773
Eigenvalues: 45.4123 127.1673 173.6679
8 C Isotropic = 59.7925 Anisotropy = 115.3847
XX= -14.6933 YX= -8.7261 ZX= 5.6801
XY= -20.1931 YY= 61.7188 ZY= -16.5785
XZ= 6.2433 YZ= -17.1515 ZZ= 132.3520
Eigenvalues: -17.3928 60.0547 136.7157
9 C Isotropic = 73.1765 Anisotropy = 112.1055
XX= 19.7109 YX= -29.1228 ZX= 0.0017
XY= -24.4200 YY= 55.6827 ZY= -20.2619
XZ= 0.8898 YZ= -15.7273 ZZ= 144.1358
Eigenvalues: 4.9630 66.6529 147.9135
10 Br Isotropic = 1910.1485 Anisotropy = 1566.6842
XX= 2790.8019 YX= 461.6684 ZX= 47.7468
XY= 475.8424 YY= 1585.6838 ZY= 39.4288
XZ= 65.0841 YZ= 54.5932 ZZ= 1353.9600
Eigenvalues: 1342.7037 1433.1373 2954.6047
11 C Isotropic = 37.1852 Anisotropy = 106.3085
XX= 28.4724 YX= -65.2451 ZX= 34.9636
XY= -67.3875 YY= 21.9684 ZY= -5.1860
XZ= 37.7207 YZ= 4.5772 ZZ= 61.1146
Eigenvalues: -47.1546 50.6526 108.0575
12 C Isotropic = 63.3178 Anisotropy = 80.5600
XX= 44.6199 YX= -1.0989 ZX= 47.9802

XY= 0.9390 YY= 100.8336 ZY= 30.1033
XZ= 39.4869 YZ= 24.6390 ZZ= 44.5000
Eigenvalues: -2.9573 75.8863 117.0245
13 O Isotropic = 22.2961 Anisotropy = 185.6809
XX= 35.3456 YX= -92.6196 ZX= 46.3427
XY= -97.0037 YY= -2.5207 ZY= -27.4416
XZ= 30.6160 YZ= -69.7840 ZZ= 34.0632
Eigenvalues: -82.0588 2.8636 146.0834
14 C Isotropic = 23.0790 Anisotropy = 84.8257
XX= 21.3758 YX= -23.0440 ZX= 51.8614
XY= -26.1179 YY= 44.0684 ZY= -1.8666
XZ= 47.0052 YZ= -14.8484 ZZ= 3.7929
Eigenvalues: -38.7664 28.3740 79.6295
15 N Isotropic = -20.5601 Anisotropy = 319.3671
XX= -14.6540 YX= -153.5446 ZX= 103.0303
XY= -153.4217 YY= -39.0629 ZY= -47.2997
XZ= 136.1190 YZ= -23.8688 ZZ= -7.9634
Eigenvalues: -200.4388 -53.5928 192.3513
16 I Isotropic = 3739.7700 Anisotropy = 2026.3922
XX= 3704.0699 YX= -192.4811 ZX= -870.6328
XY= -252.7309 YY= 2938.2220 ZY= -137.7389
XZ= -816.6689 YZ= -75.9050 ZZ= 4577.0181
Eigenvalues: 2788.0359 3340.5760 5090.6981
17 N Isotropic = 98.8848 Anisotropy = 124.6581
XX= 128.8332 YX= -16.4557 ZX= 51.2524
XY= -14.4372 YY= 110.9565 ZY= -55.7116
XZ= 52.2238 YZ= -55.2943 ZZ= 56.8646
Eigenvalues: 10.2122 104.4520 181.9902
18 C Isotropic = 62.0256 Anisotropy = 98.8744
XX= 74.4685 YX= -47.7014 ZX= 19.4362
XY= -50.9732 YY= 39.1056 ZY= -27.5610
XZ= 15.7441 YZ= -32.7315 ZZ= 72.5026
Eigenvalues: 0.9851 57.1499 127.9418
19 C Isotropic = 70.3634 Anisotropy = 142.9155
XX= 101.9324 YX= -43.3127 ZX= 36.7079
XY= -44.6590 YY= 54.7519 ZY= -59.4296
XZ= 37.9143 YZ= -58.7202 ZZ= 54.4059
Eigenvalues: -4.7690 50.2187 165.6404
20 C Isotropic = 70.9729 Anisotropy = 137.0254
XX= 70.0882 YX= -50.8406 ZX= 65.2875
XY= -52.9327 YY= 81.9938 ZY= -16.6794
XZ= 64.3435 YZ= -17.3690 ZZ= 60.8367
Eigenvalues: -6.9038 57.4993 162.3231
21 C Isotropic = 63.5974 Anisotropy = 117.0599
XX= 66.4291 YX= -66.6124 ZX= 26.9420
XY= -63.4465 YY= 42.0534 ZY= -23.0647
XZ= 30.1708 YZ= -19.2495 ZZ= 82.3098
Eigenvalues: -11.9657 61.1206 141.6374
22 H Isotropic = 24.1766 Anisotropy = 10.5410
XX= 26.8170 YX= 4.1439 ZX= 1.1531
XY= 3.3889 YY= 27.0006 ZY= 2.3047
XZ= 1.5326 YZ= 2.2349 ZZ= 18.7123
Eigenvalues: 18.1122 23.2137 31.2039
23 H Isotropic = 24.1183 Anisotropy = 9.8295
XX= 30.2563 YX= -1.6355 ZX= -0.9489
XY= -1.1335 YY= 23.9365 ZY= 1.8770
XZ= -0.8023 YZ= 1.7792 ZZ= 18.1622
Eigenvalues: 17.6152 24.0685 30.6713

 24 H Isotropic = 23.7069 Anisotropy = 11.0420
XX= 29.7818 YX= 1.1105 ZX= 2.7448
XY= 0.3629 YY= 20.7556 ZY= 2.1249
XZ= 3.9577 YZ= 2.3674 ZZ= 20.5833
Eigenvalues: 18.0607 21.9917 31.0682
 25 H Isotropic = 23.9734 Anisotropy = 9.9341
XX= 25.3885 YX= -0.5075 ZX= -0.8558
XY= 0.3599 YY= 29.4189 ZY= 3.7609
XZ= -0.8633 YZ= 4.1372 ZZ= 17.1127
Eigenvalues: 15.8864 25.4377 30.5961
 26 H Isotropic = 24.2134 Anisotropy = 5.9241
XX= 24.9473 YX= 0.4735 ZX= -1.0507
XY= -0.5050 YY= 27.6024 ZY= 2.7011
XZ= -0.8208 YZ= 1.4709 ZZ= 20.0905
Eigenvalues: 19.4032 25.0742 28.1628
 27 H Isotropic = 23.1230 Anisotropy = 7.8313
XX= 22.4373 YX= 3.9438 ZX= -4.8856
XY= 3.9877 YY= 22.7580 ZY= 2.6435
XZ= -4.8995 YZ= 2.7543 ZZ= 24.1737
Eigenvalues: 15.2820 25.7431 28.3439
 28 H Isotropic = 24.3454 Anisotropy = 5.4492
XX= 24.7171 YX= 2.6024 ZX= -2.4125
XY= 2.4253 YY= 24.1690 ZY= 0.6087
XZ= -3.0290 YZ= 0.1705 ZZ= 24.1503
Eigenvalues: 20.5093 24.5488 27.9783
 29 H Isotropic = 25.1064 Anisotropy = 2.4265
XX= 24.8465 YX= 1.3254 ZX= -1.5827
XY= 1.6807 YY= 25.3190 ZY= 0.8052
XZ= -1.3904 YZ= 1.0114 ZZ= 25.1536
Eigenvalues: 22.4567 26.1384 26.7240
 30 H Isotropic = 24.7285 Anisotropy = 3.5759
XX= 24.5361 YX= 1.8825 ZX= -2.0178
XY= 2.4975 YY= 25.1333 ZY= 0.7036
XZ= -1.4335 YZ= 1.4074 ZZ= 24.5161
Eigenvalues: 21.3574 25.7157 27.1124

Isomer 4 (conformer 1)

1 C Isotropic = 56.6364 Anisotropy = 145.8454
XX= -39.6511 YX= 0.0000 ZX= 16.9782
XY= 0.0000 YY= 153.8667 ZY= 0.0000
XZ= 13.6741 YZ= 0.0000 ZZ= 55.6937
Eigenvalues: -42.0541 58.0967 153.8667
2 C Isotropic = 47.1693 Anisotropy = 114.1488
XX= 54.9859 YX= 0.0000 ZX= 20.4861
XY= 0.0000 YY= 123.2684 ZY= 0.0000
XZ= 24.4574 YZ= 0.0000 ZZ= -36.7466
Eigenvalues: -41.9557 60.1950 123.2684
3 C Isotropic = 69.5756 Anisotropy = 126.2057
XX= 37.6170 YX= 0.0000 ZX= -38.0604
XY= 0.0000 YY= 153.7127 ZY= 0.0000
XZ= -33.8760 YZ= 0.0000 ZZ= 17.3970
Eigenvalues: -9.8551 64.8691 153.7127
4 C Isotropic = 46.6691 Anisotropy = 137.6021
XX= -28.5098 YX= 0.0000 ZX= 9.9574
XY= 0.0000 YY= 138.4039 ZY= 0.0000
XZ= 9.3511 YZ= 0.0000 ZZ= 30.1133
Eigenvalues: -30.0588 31.6623 138.4039
5 C Isotropic = 59.4380 Anisotropy = 164.3463
XX= 21.5176 YX= 0.0000 ZX= 2.2959
XY= 0.0000 YY= 169.0022 ZY= 0.0000
XZ= 1.3514 YZ= 0.0000 ZZ= -12.2058
Eigenvalues: -12.3042 21.6160 169.0022
6 C Isotropic = 59.5391 Anisotropy = 171.7668
XX= -10.3936 YX= 0.0000 ZX= -33.2850
XY= 0.0000 YY= 174.0504 ZY= 0.0000
XZ= -37.9216 YZ= 0.0000 ZZ= 14.9606
Eigenvalues: -35.5094 40.0764 174.0504
7 N Isotropic = 113.3594 Anisotropy = 89.0829
XX= 58.0664 YX= 0.0000 ZX= -36.5655
XY= 0.0000 YY= 172.7480 ZY= 0.0000
XZ= -26.2334 YZ= 0.0000 ZZ= 109.2638
Eigenvalues: 43.1532 124.1771 172.7480
8 C Isotropic = 59.9728 Anisotropy = 117.7678
XX= 41.4399 YX= 0.0000 ZX= 20.5093
XY= 0.0000 YY= 138.4846 ZY= 0.0000
XZ= 34.3201 YZ= 0.0000 ZZ= -0.0062
Eigenvalues: -13.6489 55.0827 138.4846
9 C Isotropic = 75.3678 Anisotropy = 105.4496
XX= 63.9419 YX= 0.0000 ZX= 12.9572
XY= 0.0000 YY= 145.6675 ZY= 0.0000
XZ= 6.4353 YZ= 0.0000 ZZ= 16.4938
Eigenvalues: 14.5888 65.8469 145.6675
10 C Isotropic = 19.6296 Anisotropy = 84.1921
XX= -23.9687 YX= 0.0000 ZX= -20.5086
XY= 0.0000 YY= 75.7576 ZY= 0.0000
XZ= -33.0164 YZ= 0.0000 ZZ= 7.0998
Eigenvalues: -39.3787 22.5098 75.7576
11 Br Isotropic = 1893.0501 Anisotropy = 1574.0629
XX= 1538.5744 YX= 0.0000 ZX= -404.9429
XY= 0.0000 YY= 1319.8455 ZY= 0.0000
XZ= -421.7170 YZ= 0.0000 ZZ= 2820.7303
Eigenvalues: 1319.8455 1416.8794 2942.4253
12 N Isotropic = -2.3899 Anisotropy = 309.7346
XX= -58.9136 YX= 0.0000 ZX= -63.3256

XY= 0.0000 YY= 204.0998 ZY= 0.0000
XZ= -34.3231 YZ= 0.0000 ZZ= -152.3560
Eigenvalues: -173.2121 -38.0575 204.0998
13 C Isotropic = 42.3812 Anisotropy = 105.9744
XX= 44.2463 YX= 0.0000 ZX= -27.8292
XY= 0.0000 YY= 113.0307 ZY= 0.0000
XZ= -18.3775 YZ= 0.0000 ZZ= -30.1335
Eigenvalues: -36.7255 50.8382 113.0307
14 C Isotropic = 67.9294 Anisotropy = 71.3328
XX= 42.6363 YX= 0.0000 ZX= -41.3140
XY= 0.0000 YY= 77.1965 ZY= 0.0000
XZ= -54.5371 YZ= 0.0000 ZZ= 83.9553
Eigenvalues: 11.1070 77.1965 115.4846
15 O Isotropic = 11.2900 Anisotropy = 189.0476
XX= -4.5694 YX= 0.0000 ZX= 27.3618
XY= 0.0000 YY= 137.3217 ZY= 0.0000
XZ= -6.0133 YZ= 0.0000 ZZ= -98.8824
Eigenvalues: -100.0754 -3.3764 137.3217
16 C Isotropic = 60.8576 Anisotropy = 105.3384
XX= 20.0723 YX= 0.0000 ZX= 31.0923
XY= 0.0000 YY= 131.0832 ZY= 0.0000
XZ= 21.8552 YZ= 0.0000 ZZ= 31.4174
Eigenvalues: -1.3298 52.8195 131.0832
17 N Isotropic = 94.8953 Anisotropy = 125.3185
XX= 35.3111 YX= 0.0000 ZX= -45.5928
XY= 0.0000 YY= 178.4409 ZY= 0.0000
XZ= -39.4169 YZ= 0.0000 ZZ= 70.9337
Eigenvalues: 7.0365 99.2083 178.4409
18 C Isotropic = 66.0229 Anisotropy = 116.4733
XX= 34.6693 YX= 0.0000 ZX= 32.1658
XY= 0.0000 YY= 143.6717 ZY= 0.0000
XZ= 42.0976 YZ= 0.0000 ZZ= 19.7276
Eigenvalues: -10.6774 65.0743 143.6717
19 C Isotropic = 71.9524 Anisotropy = 133.2865
XX= 61.4068 YX= 0.0000 ZX= -4.4145
XY= 0.0000 YY= 160.8101 ZY= 0.0000
XZ= -8.9048 YZ= 0.0000 ZZ= -6.3596
Eigenvalues: -7.0079 62.0550 160.8101
20 C Isotropic = 73.8995 Anisotropy = 138.1672
XX= 1.6318 YX= 0.0000 ZX= -3.5196
XY= 0.0000 YY= 166.0109 ZY= 0.0000
XZ= -5.1178 YZ= 0.0000 ZZ= 54.0556
Eigenvalues: 1.2785 54.4090 166.0109
21 I Isotropic = 3663.1528 Anisotropy = 1983.2448
XX= 4765.3997 YX= 0.0000 ZX= 691.2500
XY= 0.0000 YY= 3278.0006 ZY= 0.0000
XZ= 648.1024 YZ= 0.0000 ZZ= 2946.0582
Eigenvalues: 2726.1419 3278.0006 4985.3161
22 H Isotropic = 24.0248 Anisotropy = 10.6849
XX= 23.5641 YX= 0.0000 ZX= 1.9678
XY= 0.0000 YY= 17.9376 ZY= 0.0000
XZ= 2.2099 YZ= 0.0000 ZZ= 30.5727
Eigenvalues: 17.9376 22.9888 31.1481
23 H Isotropic = 24.1816 Anisotropy = 10.0145
XX= 27.9435 YX= 0.0000 ZX= -3.0585
XY= 0.0000 YY= 17.7582 ZY= 0.0000
XZ= -3.7828 YZ= 0.0000 ZZ= 26.8431
Eigenvalues: 17.7582 23.9287 30.8579

24 H Isotropic = 23.1173 Anisotropy = 11.0309
XX= 23.8914 YX= 0.0000 ZX= -1.6962
XY= 0.0000 YY= 15.5939 ZY= 0.0000
XZ= -2.2928 YZ= 0.0000 ZZ= 29.8666
Eigenvalues: 15.5939 23.2868 30.4712
25 H Isotropic = 23.9149 Anisotropy = 9.3323
XX= 28.8413 YX= 0.0000 ZX= 2.3192
XY= 0.0000 YY= 15.7399 ZY= 0.0000
XZ= 1.6054 YZ= 0.0000 ZZ= 27.1637
Eigenvalues: 15.7399 25.8684 30.1365
26 H Isotropic = 23.6972 Anisotropy = 5.8639
XX= 26.0618 YX= 0.0000 ZX= 0.1817
XY= 0.0000 YY= 18.1514 ZY= 0.0000
XZ= 1.9392 YZ= 0.0000 ZZ= 26.8784
Eigenvalues: 18.1514 25.3338 27.6065
27 H Isotropic = 22.9135 Anisotropy = 8.1060
XX= 26.9496 YX= 0.0000 ZX= 1.0394
XY= 0.0000 YY= 14.3497 ZY= 0.0000
XZ= 1.1504 YZ= 0.0000 ZZ= 27.4411
Eigenvalues: 14.3497 26.0732 28.3175
28 H Isotropic = 24.6839 Anisotropy = 3.5161
XX= 26.3111 YX= 0.0000 ZX= -1.2108
XY= 0.0000 YY= 21.1998 ZY= 0.0000
XZ= 0.0289 YZ= 0.0000 ZZ= 26.5407
Eigenvalues: 21.1998 25.8239 27.0279
29 H Isotropic = 25.1520 Anisotropy = 3.0910
XX= 26.4261 YX= 0.0000 ZX= -0.7866
XY= 0.0000 YY= 22.2017 ZY= 0.0000
XZ= -0.3133 YZ= 0.0000 ZZ= 26.8281
Eigenvalues: 22.2017 26.0416 27.2126
30 H Isotropic = 24.3634 Anisotropy = 11.8438
XX= 24.8136 YX= 0.0000 ZX= -4.0617
XY= 0.0000 YY= 17.9251 ZY= 0.0000
XZ= -3.4763 YZ= 0.0000 ZZ= 30.3515
Eigenvalues: 17.9251 22.9058 32.2593

Isomer 4 (conformer 2)

```
  1 C   Isotropic =   57.1684   Anisotropy =  145.1603
XX=  -35.9977   YX=    0.0000   ZX=   23.0109
XY=    0.0000   YY=  153.9419   ZY=    0.0000
XZ=   19.3386   YZ=    0.0000   ZZ=   53.5611
Eigenvalues:  -40.7518   58.3152  153.9419
  2 C   Isotropic =   47.0701   Anisotropy =  113.8365
XX=   57.7544   YX=    0.0000   ZX=   14.0376
XY=    0.0000   YY=  122.9611   ZY=    0.0000
XZ=   18.0390   YZ=    0.0000   ZZ=  -39.5053
Eigenvalues:  -42.0818   60.3309  122.9611
  3 C   Isotropic =   69.6738   Anisotropy =  126.2778
XX=   32.8458   YX=    0.0000   ZX=  -39.6019
XY=    0.0000   YY=  153.8590   ZY=    0.0000
XZ=  -34.7228   YZ=    0.0000   ZZ=   22.3166
Eigenvalues:   -9.9522   65.1146  153.8590
  4 C   Isotropic =   46.4661   Anisotropy =  138.3038
XX=  -27.4378   YX=    0.0000   ZX=   13.9958
XY=    0.0000   YY=  138.6687   ZY=    0.0000
XZ=   13.5675   YZ=    0.0000   ZZ=   28.1675
Eigenvalues:  -30.6661   31.3958  138.6687
  5 C   Isotropic =   59.4899   Anisotropy =  163.9445
XX=   22.4194   YX=    0.0000   ZX=   -0.6026
XY=    0.0000   YY=  168.7862   ZY=    0.0000
XZ=   -0.4792   YZ=    0.0000   ZZ=  -12.7361
Eigenvalues:  -12.7444   22.4278  168.7862
  6 C   Isotropic =   59.0484   Anisotropy =  173.8719
XX=  -15.7763   YX=    0.0000   ZX=  -31.3481
XY=    0.0000   YY=  174.9630   ZY=    0.0000
XZ=  -35.8327   YZ=    0.0000   ZZ=   17.9585
Eigenvalues:  -36.4965   38.6786  174.9630
  7 N   Isotropic =  114.0381   Anisotropy =   87.6321
XX=   55.8725   YX=    0.0000   ZX=  -32.7009
XY=    0.0000   YY=  172.4595   ZY=    0.0000
XZ=  -20.4012   YZ=    0.0000   ZZ=  113.7822
Eigenvalues:   45.5420  124.1127  172.4595
  8 C   Isotropic =   59.9395   Anisotropy =  118.0960
XX=   44.0051   YX=    0.0000   ZX=   16.0413
XY=    0.0000   YY=  138.6702   ZY=    0.0000
XZ=   32.1471   YZ=    0.0000   ZZ=   -2.8567
Eigenvalues:  -13.0344   54.1828  138.6702
  9 C   Isotropic =   75.3350   Anisotropy =  105.8546
XX=   63.2318   YX=    0.0000   ZX=    8.7968
XY=    0.0000   YY=  145.9048   ZY=    0.0000
XZ=    0.6966   YZ=    0.0000   ZZ=   16.8686
Eigenvalues:   16.3876   63.7128  145.9048
 10 C   Isotropic =   20.5002   Anisotropy =   85.2011
XX=   20.5858   YX=    0.0000   ZX=    6.9506
XY=    0.0000   YY=   77.3010   ZY=    0.0000
XZ=   19.0366   YZ=    0.0000   ZZ=  -36.3860
Eigenvalues:  -39.2096   23.4093   77.3010
 11 Br   Isotropic = 1891.8746   Anisotropy = 1573.2670
XX= 1489.9234   YX=    0.0000   ZX= -313.2970
XY=    0.0000   YY= 1316.9035   ZY=    0.0000
XZ= -332.7516   YZ=    0.0000   ZZ= 2868.7969
Eigenvalues: 1316.9035 1418.0010 2940.7193
 12 N   Isotropic =   -7.0221   Anisotropy =  319.5960
XX=  -77.7820   YX=    0.0000   ZX=  -48.9990
```

XY= 0.0000 YY= 206.0419 ZY= 0.0000
XZ= -63.0125 YZ= 0.0000 ZZ= -149.3263
Eigenvalues: -180.0093 -47.0990 206.0419
13 C Isotropic = 41.9902 Anisotropy = 106.1535
XX= 25.7668 YX= 0.0000 ZX= -34.8068
XY= 0.0000 YY= 112.7592 ZY= 0.0000
XZ= -44.0681 YZ= 0.0000 ZZ= -12.5554
Eigenvalues: -37.2402 50.4516 112.7592
14 C Isotropic = 67.3982 Anisotropy = 70.3723
XX= 112.4378 YX= 0.0000 ZX= 7.8574
XY= 0.0000 YY= 76.6665 ZY= 0.0000
XZ= 19.6972 YZ= 0.0000 ZZ= 13.0903
Eigenvalues: 11.2151 76.6665 114.3130
15 O Isotropic = 17.6490 Anisotropy = 169.6531
XX= -60.8696 YX= 0.0000 ZX= -73.5872
XY= 0.0000 YY= 130.7510 ZY= 0.0000
XZ= -32.1693 YZ= 0.0000 ZZ= -16.9345
Eigenvalues: -96.1619 18.3577 130.7510
16 C Isotropic = 61.0622 Anisotropy = 106.2851
XX= -0.4643 YX= 0.0000 ZX= 3.4039
XY= 0.0000 YY= 131.9189 ZY= 0.0000
XZ= 12.1575 YZ= 0.0000 ZZ= 51.7321
Eigenvalues: -1.5995 52.8672 131.9189
17 N Isotropic = 95.7617 Anisotropy = 123.8644
XX= 99.7452 YX= 0.0000 ZX= 17.1258
XY= 0.0000 YY= 178.3380 ZY= 0.0000
XZ= 10.6265 YZ= 0.0000 ZZ= 9.2020
Eigenvalues: 7.1231 101.8241 178.3380
18 C Isotropic = 65.9569 Anisotropy = 115.6720
XX= -9.8851 YX= 0.0000 ZX= 1.0962
XY= 0.0000 YY= 143.0716 ZY= 0.0000
XZ= -9.3457 YZ= 0.0000 ZZ= 64.6843
Eigenvalues: -10.1126 64.9118 143.0716
19 C Isotropic = 71.5654 Anisotropy = 133.2593
XX= 30.0247 YX= 0.0000 ZX= -36.1295
XY= 0.0000 YY= 160.4049 ZY= 0.0000
XZ= -31.4242 YZ= 0.0000 ZZ= 24.2665
Eigenvalues: -6.7537 61.0449 160.4049
20 C Isotropic = 73.8020 Anisotropy = 138.6932
XX= 32.9126 YX= 0.0000 ZX= 23.3945
XY= 0.0000 YY= 166.2642 ZY= 0.0000
XZ= 25.9700 YZ= 0.0000 ZZ= 22.2293
Eigenvalues: 2.3173 52.8246 166.2642
21 I Isotropic = 3678.8351 Anisotropy = 1987.8749
XX= 3092.1047 YX= 0.0000 ZX= -857.6764
XY= 0.0000 YY= 3315.3729 ZY= 0.0000
XZ= -835.9612 YZ= 0.0000 ZZ= 4629.0277
Eigenvalues: 2717.0474 3315.3729 5004.0850
22 H Isotropic = 24.0362 Anisotropy = 10.3698
XX= 24.0863 YX= 0.0000 ZX= 2.3205
XY= 0.0000 YY= 17.9620 ZY= 0.0000
XZ= 2.6197 YZ= 0.0000 ZZ= 30.0604
Eigenvalues: 17.9620 23.1973 30.9494
23 H Isotropic = 24.1892 Anisotropy = 10.0553
XX= 27.4713 YX= 0.0000 ZX= -3.1596
XY= 0.0000 YY= 17.7874 ZY= 0.0000
XZ= -3.8438 YZ= 0.0000 ZZ= 27.3089
Eigenvalues: 17.7874 23.8874 30.8928

24 H Isotropic = 22.9380 Anisotropy = 10.2409
XX= 24.2310 YX= 0.0000 ZX= -1.7605
XY= 0.0000 YY= 15.5180 ZY= 0.0000
XZ= -2.1764 YZ= 0.0000 ZZ= 29.0651
Eigenvalues: 15.5180 23.5308 29.7653
25 H Isotropic = 23.9621 Anisotropy = 9.2889
XX= 29.0084 YX= 0.0000 ZX= 2.1203
XY= 0.0000 YY= 15.8305 ZY= 0.0000
XZ= 1.6542 YZ= 0.0000 ZZ= 27.0474
Eigenvalues: 15.8305 25.9011 30.1547
26 H Isotropic = 23.8382 Anisotropy = 6.7428
XX= 26.0788 YX= 0.0000 ZX= 0.5607
XY= 0.0000 YY= 18.0943 ZY= 0.0000
XZ= 2.4302 YZ= 0.0000 ZZ= 27.3415
Eigenvalues: 18.0943 25.0869 28.3334
27 H Isotropic = 22.6643 Anisotropy = 8.7459
XX= 25.8314 YX= 0.0000 ZX= 0.7814
XY= 0.0000 YY= 13.8468 ZY= 0.0000
XZ= 0.6040 YZ= 0.0000 ZZ= 28.3148
Eigenvalues: 13.8468 25.6512 28.4950
28 H Isotropic = 24.7372 Anisotropy = 3.5417
XX= 27.0920 YX= 0.0000 ZX= 0.7668
XY= 0.0000 YY= 20.9610 ZY= 0.0000
XZ= -0.6118 YZ= 0.0000 ZZ= 26.1587
Eigenvalues: 20.9610 26.1523 27.0984
29 H Isotropic = 25.1314 Anisotropy = 2.9977
XX= 27.1017 YX= 0.0000 ZX= 0.4021
XY= 0.0000 YY= 22.0693 ZY= 0.0000
XZ= -0.0824 YZ= 0.0000 ZZ= 26.2232
Eigenvalues: 22.0693 26.1950 27.1299
30 H Isotropic = 24.4061 Anisotropy = 11.6796
XX= 31.5617 YX= 0.0000 ZX= 2.5158
XY= 0.0000 YY= 17.7671 ZY= 0.0000
XZ= 2.0612 YZ= 0.0000 ZZ= 23.8893
Eigenvalues: 17.7671 23.2586 32.1925

Isomer 4 (conformer 3)

```
  1  C    Isotropic =    56.6571   Anisotropy =   145.7821
 XX=   -39.6708   YX=     0.0000   ZX=    17.7890
 XY=     0.0000   YY=   153.8451   ZY=     0.0000
 XZ=    14.3524   YZ=     0.0000   ZZ=    55.7969
 Eigenvalues:   -42.3035    58.4296   153.8451
  2  C    Isotropic =    47.5728   Anisotropy =   113.7713
 XX=    55.8447   YX=     0.0000   ZX=    20.0226
 XY=     0.0000   YY=   123.4203   ZY=     0.0000
 XZ=    23.9248   YZ=     0.0000   ZZ=   -36.5466
 Eigenvalues:   -41.5064    60.8045   123.4203
  3  C    Isotropic =    69.6473   Anisotropy =   126.3618
 XX=    37.2192   YX=     0.0000   ZX=   -38.2124
 XY=     0.0000   YY=   153.8885   ZY=     0.0000
 XZ=   -33.9863   YZ=     0.0000   ZZ=    17.8343
 Eigenvalues:    -9.8511    64.9046   153.8885
  4  C    Isotropic =    46.6318   Anisotropy =   137.4154
 XX=   -28.2388   YX=     0.0000   ZX=    10.2998
 XY=     0.0000   YY=   138.2420   ZY=     0.0000
 XZ=     9.5658   YZ=     0.0000   ZZ=    29.8920
 Eigenvalues:   -29.8892    31.5424   138.2420
  5  C    Isotropic =    59.2648   Anisotropy =   164.8220
 XX=    21.0749   YX=     0.0000   ZX=     1.7331
 XY=     0.0000   YY=   169.1461   ZY=     0.0000
 XZ=     1.0661   YZ=     0.0000   ZZ=   -12.4267
 Eigenvalues:   -12.4851    21.1333   169.1461
  6  C    Isotropic =    59.6518   Anisotropy =   171.2929
 XX=   -10.5347   YX=     0.0000   ZX=   -33.4824
 XY=     0.0000   YY=   173.8471   ZY=     0.0000
 XZ=   -37.9053   YZ=     0.0000   ZZ=    15.6430
 Eigenvalues:   -35.4638    40.5722   173.8471
  7  N    Isotropic =   112.9007   Anisotropy =    89.5364
 XX=    56.6646   YX=     0.0000   ZX=   -36.1747
 XY=     0.0000   YY=   172.5917   ZY=     0.0000
 XZ=   -25.8928   YZ=     0.0000   ZZ=   109.4460
 Eigenvalues:    42.3175   123.7931   172.5917
  8  C    Isotropic =    59.0367   Anisotropy =   119.5157
 XX=    40.5612   YX=     0.0000   ZX=    19.8481
 XY=     0.0000   YY=   138.7138   ZY=     0.0000
 XZ=    33.5027   YZ=     0.0000   ZZ=    -2.1650
 Eigenvalues:   -14.9773    53.3735   138.7138
  9  C    Isotropic =    75.4433   Anisotropy =   105.0128
 XX=    64.2972   YX=     0.0000   ZX=    12.6734
 XY=     0.0000   YY=   145.4518   ZY=     0.0000
 XZ=     6.2027   YZ=     0.0000   ZZ=    16.5809
 Eigenvalues:    14.7819    66.0962   145.4518
 10  C    Isotropic =    18.8774   Anisotropy =    84.1731
 XX=   -26.3556   YX=     0.0000   ZX=   -21.5287
 XY=     0.0000   YY=    74.9928   ZY=     0.0000
 XZ=   -35.7759   YZ=     0.0000   ZZ=     7.9949
 Eigenvalues:   -42.5861    24.2254    74.9928
 11  Br   Isotropic =  1896.3345   Anisotropy =  1571.4629
 XX=  1539.4230   YX=     0.0000   ZX=  -394.9038
 XY=     0.0000   YY=  1321.4948   ZY=     0.0000
 XZ=  -412.0025   YZ=     0.0000   ZZ=  2828.0859
 Eigenvalues:  1321.4948  1423.5324  2943.9765
 12  N    Isotropic =   -12.0254   Anisotropy =   316.1235
 XX=   -64.3973   YX=     0.0000   ZX=   -65.0517
```

XY= 0.0000 YY= 198.7236 ZY= 0.0000
XZ= -37.1601 YZ= 0.0000 ZZ= -170.4024
Eigenvalues: -191.0279 -43.7718 198.7236
13 C Isotropic = 41.6153 Anisotropy = 108.2623
XX= 43.0032 YX= 0.0000 ZX= -27.4526
XY= 0.0000 YY= 113.7902 ZY= 0.0000
XZ= -19.4427 YZ= 0.0000 ZZ= -31.9473
Eigenvalues: -38.6782 49.7341 113.7902
14 C Isotropic = 75.1657 Anisotropy = 83.9899
XX= 44.5706 YX= 0.0000 ZX= -42.7726
XY= 0.0000 YY= 79.1370 ZY= 0.0000
XZ= -58.0847 YZ= 0.0000 ZZ= 101.7895
Eigenvalues: 15.2012 79.1370 131.1589
15 O Isotropic = 16.4235 Anisotropy = 177.3830
XX= 7.8291 YX= 0.0000 ZX= 23.5417
XY= 0.0000 YY= 134.6789 ZY= 0.0000
XZ= -7.5018 YZ= 0.0000 ZZ= -93.2374
Eigenvalues: -93.8698 8.4616 134.6789
16 C Isotropic = 60.1767 Anisotropy = 102.9272
XX= 49.3371 YX= 0.0000 ZX= -21.4790
XY= 0.0000 YY= 128.7948 ZY= 0.0000
XZ= -16.0805 YZ= 0.0000 ZZ= 2.3981
Eigenvalues: -4.1906 55.9258 128.7948
17 N Isotropic = 98.2491 Anisotropy = 130.2242
XX= 13.8287 YX= 0.0000 ZX= -2.1127
XY= 0.0000 YY= 185.0652 ZY= 0.0000
XZ= -6.0161 YZ= 0.0000 ZZ= 95.8534
Eigenvalues: 13.6278 96.0543 185.0652
18 C Isotropic = 65.1318 Anisotropy = 113.2523
XX= 66.0569 YX= 0.0000 ZX= -0.4826
XY= 0.0000 YY= 140.6334 ZY= 0.0000
XZ= -12.7995 YZ= 0.0000 ZZ= -11.2948
Eigenvalues: -11.8608 66.6229 140.6334
19 C Isotropic = 72.6448 Anisotropy = 136.8430
XX= 33.6390 YX= 0.0000 ZX= 31.0206
XY= 0.0000 YY= 163.8735 ZY= 0.0000
XZ= 34.6393 YZ= 0.0000 ZZ= 20.4220
Eigenvalues: -6.4580 60.5190 163.8735
20 C Isotropic = 71.1151 Anisotropy = 137.4867
XX= 12.0843 YX= 0.0000 ZX= -27.0832
XY= 0.0000 YY= 162.7729 ZY= 0.0000
XZ= -24.1921 YZ= 0.0000 ZZ= 38.4880
Eigenvalues: -3.5509 54.1232 162.7729
21 I Isotropic = 3723.4127 Anisotropy = 1931.2693
XX= 4774.7061 YX= 0.0000 ZX= 704.9707
XY= 0.0000 YY= 3389.9361 ZY= 0.0000
XZ= 671.5437 YZ= 0.0000 ZZ= 3005.5960
Eigenvalues: 2769.3765 3389.9361 5010.9256
22 H Isotropic = 24.0579 Anisotropy = 10.6927
XX= 23.6123 YX= 0.0000 ZX= 2.0116
XY= 0.0000 YY= 17.9824 ZY= 0.0000
XZ= 2.2784 YZ= 0.0000 ZZ= 30.5789
Eigenvalues: 17.9824 23.0048 31.1864
23 H Isotropic = 24.1905 Anisotropy = 10.0047
XX= 27.9279 YX= 0.0000 ZX= -3.0742
XY= 0.0000 YY= 17.7811 ZY= 0.0000
XZ= -3.7736 YZ= 0.0000 ZZ= 26.8626
Eigenvalues: 17.7811 23.9302 30.8603

24 H Isotropic = 23.1846 Anisotropy = 10.9786
XX= 23.9036 YX= 0.0000 ZX= -1.7013
XY= 0.0000 YY= 15.7263 ZY= 0.0000
XZ= -2.2107 YZ= 0.0000 ZZ= 29.9240
Eigenvalues: 15.7263 23.3239 30.5037
25 H Isotropic = 23.9059 Anisotropy = 9.3373
XX= 28.8758 YX= 0.0000 ZX= 2.2902
XY= 0.0000 YY= 15.7475 ZY= 0.0000
XZ= 1.6140 YZ= 0.0000 ZZ= 27.0943
Eigenvalues: 15.7475 25.8393 30.1307
26 H Isotropic = 23.6276 Anisotropy = 5.7772
XX= 26.0293 YX= 0.0000 ZX= 0.1640
XY= 0.0000 YY= 18.1140 ZY= 0.0000
XZ= 1.9069 YZ= 0.0000 ZZ= 26.7394
Eigenvalues: 18.1140 25.2897 27.4790
27 H Isotropic = 22.3847 Anisotropy = 17.3495
XX= 27.7933 YX= 0.0000 ZX= -6.3910
XY= 0.0000 YY= 10.8693 ZY= 0.0000
XZ= -5.2053 YZ= 0.0000 ZZ= 28.4914
Eigenvalues: 10.8693 22.3337 33.9510
28 H Isotropic = 24.7674 Anisotropy = 4.0206
XX= 26.0593 YX= 0.0000 ZX= 0.1245
XY= 0.0000 YY= 21.0146 ZY= 0.0000
XZ= -1.2285 YZ= 0.0000 ZZ= 27.2284
Eigenvalues: 21.0146 25.8399 27.4478
29 H Isotropic = 25.2162 Anisotropy = 2.5531
XX= 26.5044 YX= 0.0000 ZX= -0.0777
XY= 0.0000 YY= 22.4492 ZY= 0.0000
XZ= -0.5303 YZ= 0.0000 ZZ= 26.6951
Eigenvalues: 22.4492 26.2812 26.9183
30 H Isotropic = 24.4569 Anisotropy = 5.5892
XX= 26.1288 YX= 0.0000 ZX= -1.6321
XY= 0.0000 YY= 19.9519 ZY= 0.0000
XZ= -1.0768 YZ= 0.0000 ZZ= 27.2900
Eigenvalues: 19.9519 25.2358 28.1831

Isomer 4 (conformer 4)

1 C Isotropic = 56.7164 Anisotropy = 145.5637
XX= -35.3673 YX= 0.0000 ZX= 25.4282
XY= 0.0000 YY= 153.7589 ZY= 0.0000
XZ= 21.9020 YZ= 0.0000 ZZ= 51.7578
Eigenvalues: -41.3803 57.7707 153.7589
2 C Isotropic = 46.7592 Anisotropy = 113.8638
XX= 58.1595 YX= 0.0000 ZX= 11.4684
XY= 0.0000 YY= 122.6684 ZY= 0.0000
XZ= 15.6689 YZ= 0.0000 ZZ= -40.5502
Eigenvalues: -42.3814 59.9906 122.6684
3 C Isotropic = 69.9731 Anisotropy = 125.5220
XX= 31.2677 YX= 0.0000 ZX= -39.8289
XY= 0.0000 YY= 153.6544 ZY= 0.0000
XZ= -35.2752 YZ= 0.0000 ZZ= 24.9971
Eigenvalues: -9.5503 65.8151 153.6544
4 C Isotropic = 46.4054 Anisotropy = 138.5074
XX= -26.9771 YX= 0.0000 ZX= 15.7094
XY= 0.0000 YY= 138.7437 ZY= 0.0000
XZ= 15.1292 YZ= 0.0000 ZZ= 27.4495
Eigenvalues: -31.0418 31.5143 138.7437
5 C Isotropic = 59.5822 Anisotropy = 164.2953
XX= 22.5422 YX= 0.0000 ZX= -1.1186
XY= 0.0000 YY= 169.1125 ZY= 0.0000
XZ= -1.4948 YZ= 0.0000 ZZ= -12.9079
Eigenvalues: -12.9560 22.5903 169.1125
6 C Isotropic = 58.3925 Anisotropy = 176.1805
XX= -18.8525 YX= 0.0000 ZX= -29.1650
XY= 0.0000 YY= 175.8462 ZY= 0.0000
XZ= -34.0507 YZ= 0.0000 ZZ= 18.1839
Eigenvalues: -36.9673 36.2987 175.8462
7 N Isotropic = 114.2142 Anisotropy = 87.7690
XX= 54.6595 YX= 0.0000 ZX= -31.1871
XY= 0.0000 YY= 172.7268 ZY= 0.0000
XZ= -18.8697 YZ= 0.0000 ZZ= 115.2561
Eigenvalues: 45.6588 124.2568 172.7268
8 C Isotropic = 60.1905 Anisotropy = 117.7511
XX= 45.5510 YX= 0.0000 ZX= 15.0006
XY= 0.0000 YY= 138.6912 ZY= 0.0001
XZ= 31.1121 YZ= 0.0000 ZZ= -3.6706
Eigenvalues: -12.7835 54.6639 138.6912
9 C Isotropic = 75.3076 Anisotropy = 105.9964
XX= 63.4264 YX= 0.0000 ZX= 7.4791
XY= 0.0000 YY= 145.9719 ZY= 0.0000
XZ= -0.8728 YZ= 0.0000 ZZ= 16.5245
Eigenvalues: 16.2930 63.6579 145.9719
10 C Isotropic = 19.9239 Anisotropy = 85.0650
XX= 22.5667 YX= 0.0000 ZX= 5.8374
XY= -0.0005 YY= 76.6339 ZY= 0.0000
XZ= 19.8624 YZ= 0.0000 ZZ= -39.4290
Eigenvalues: -41.9868 25.1245 76.6339
11 Br Isotropic = 1892.1319 Anisotropy = 1571.9932
XX= 1475.5332 YX= -0.0001 ZX= -276.9825
XY= 0.0002 YY= 1316.5462 ZY= 0.0000
XZ= -294.8234 YZ= 0.0001 ZZ= 2884.3164
Eigenvalues: 1316.5462 1419.7222 2940.1274
12 N Isotropic = -15.8325 Anisotropy = 326.1184
XX= -91.1108 YX= -0.0002 ZX= -58.6706

XY= 0.0026 YY= 201.5797 ZY= 0.0012
XZ= -70.5900 YZ= 0.0004 ZZ= -157.9664
Eigenvalues: -197.3019 -51.7754 201.5797
13 C Isotropic = 41.3247 Anisotropy = 108.2499
XX= 22.5878 YX= -0.0008 ZX= -37.0301
XY= 0.0007 YY= 113.4914 ZY= -0.0003
XZ= -44.3916 YZ= -0.0009 ZZ= -12.1049
Eigenvalues: -39.0110 49.4938 113.4914
14 C Isotropic = 74.7040 Anisotropy = 82.6122
XX= 126.7167 YX= -0.0004 ZX= 11.4155
XY= 0.0077 YY= 79.1065 ZY= 0.0062
XZ= 25.5383 YZ= 0.0001 ZZ= 18.2888
Eigenvalues: 15.2267 79.1065 129.7788
15 O Isotropic = 23.4975 Anisotropy = 158.6400
XX= -52.8248 YX= -0.0005 ZX= -74.8163
XY= -0.0004 YY= 129.2575 ZY= -0.0003
XZ= -35.9106 YZ= 0.0001 ZZ= -5.9402
Eigenvalues: -89.5045 30.7395 129.2575
16 C Isotropic = 60.0429 Anisotropy = 103.7312
XX= 40.7760 YX= -0.0044 ZX= -24.1384
XY= -0.0152 YY= 129.1970 ZY= -0.0268
XZ= -28.8091 YZ= 0.0010 ZZ= 10.1556
Eigenvalues: -5.1162 56.0479 129.1970
17 N Isotropic = 96.7538 Anisotropy = 132.2398
XX= 62.7282 YX= 0.0032 ZX= 36.8842
XY= -0.0229 YY= 184.9136 ZY= 0.0551
XZ= 39.9429 YZ= -0.0018 ZZ= 42.6196
Eigenvalues: 12.9663 92.3814 184.9137
18 C Isotropic = 65.5322 Anisotropy = 112.5196
XX= 29.5609 YX= 0.0058 ZX= -45.6969
XY= 0.0457 YY= 140.5453 ZY= 0.0541
XZ= -33.4888 YZ= -0.0076 ZZ= 26.4905
Eigenvalues: -11.5970 67.6483 140.5453
19 C Isotropic = 72.8275 Anisotropy = 137.6432
XX= -6.7457 YX= 0.0904 ZX= -0.1013
XY= 0.0368 YY= 164.5896 ZY= 0.0007
XZ= -3.7518 YZ= -0.0014 ZZ= 60.6385
Eigenvalues: -6.8008 60.6936 164.5896
20 C Isotropic = 70.4945 Anisotropy = 137.7592
XX= 52.4733 YX= 0.0110 ZX= 11.7186
XY= 0.0308 YY= 162.3339 ZY= -0.0655
XZ= 9.4481 YZ= 0.0039 ZZ= -3.3238
Eigenvalues: -5.2638 54.4133 162.3340
21 I Isotropic = 3733.5418 Anisotropy = 1973.0647
XX= 3090.6699 YX= 0.0073 ZX= -785.4217
XY= -0.0276 YY= 3373.4705 ZY= 0.0130
XZ= -778.9593 YZ= -0.0004 ZZ= 4736.4850
Eigenvalues: 2778.2366 3373.4705 5048.9183
22 H Isotropic = 24.0212 Anisotropy = 10.3222
XX= 24.2478 YX= 0.0000 ZX= 2.5021
XY= 0.0000 YY= 17.9615 ZY= 0.0000
XZ= 2.7805 YZ= 0.0000 ZZ= 29.8543
Eigenvalues: 17.9615 23.1995 30.9027
23 H Isotropic = 24.2281 Anisotropy = 10.0998
XX= 27.3214 YX= 0.0000 ZX= -3.1954
XY= 0.0000 YY= 17.8272 ZY= 0.0000
XZ= -3.8669 YZ= 0.0000 ZZ= 27.5356
Eigenvalues: 17.8272 23.8958 30.9613

 24 H Isotropic = 22.8691 Anisotropy = 10.1180
XX= 24.1072 YX= 0.0000 ZX= -1.6823
XY= -0.0001 YY= 15.5323 ZY= 0.0000
XZ= -2.0922 YZ= 0.0000 ZZ= 28.9676
Eigenvalues: 15.5323 23.4605 29.6144
 25 H Isotropic = 24.0083 Anisotropy = 9.1962
XX= 29.0767 YX= 0.0000 ZX= 2.0582
XY= 0.0000 YY= 15.9388 ZY= 0.0000
XZ= 1.5887 YZ= 0.0000 ZZ= 27.0093
Eigenvalues: 15.9388 25.9470 30.1390
 26 H Isotropic = 23.9178 Anisotropy = 6.7081
XX= 26.1692 YX= 0.0000 ZX= 0.6189
XY= 0.0000 YY= 18.2410 ZY= 0.0000
XZ= 2.4302 YZ= 0.0000 ZZ= 27.3432
Eigenvalues: 18.2410 25.1225 28.3899
 27 H Isotropic = 22.3949 Anisotropy = 17.6219
XX= 34.1104 YX= -0.0001 ZX= -0.0762
XY= -0.0015 YY= 10.4603 ZY= 0.0010
XZ= -1.1479 YZ= 0.0000 ZZ= 22.6141
Eigenvalues: 10.4603 22.5816 34.1429
 28 H Isotropic = 24.6508 Anisotropy = 3.9767
XX= 27.0744 YX= -0.0003 ZX= -0.0328
XY= 0.0017 YY= 20.9488 ZY= 0.0012
XZ= 1.1505 YZ= 0.0000 ZZ= 25.9294
Eigenvalues: 20.9488 25.7018 27.3020
 29 H Isotropic = 25.1376 Anisotropy = 2.4430
XX= 26.7520 YX= 0.0018 ZX= -0.1560
XY= -0.0059 YY= 22.2807 ZY= 0.0001
XZ= 0.3048 YZ= -0.0001 ZZ= 26.3801
Eigenvalues: 22.2807 26.3658 26.7663
 30 H Isotropic = 24.2970 Anisotropy = 5.5051
XX= 27.8070 YX= -0.0003 ZX= 0.8700
XY= 0.0011 YY= 19.5958 ZY= -0.0021
XZ= 0.3898 YZ= 0.0000 ZZ= 25.4883
Eigenvalues: 19.5958 25.3282 27.9671

Isomer 5 (conformer 1)

1 C Isotropic = 56.4680 Anisotropy = 145.7535
XX= -41.8011 YX= 7.8172 ZX= -4.2552
XY= 7.7767 YY= 152.9670 ZY= -5.6876
XZ= -1.9282 YZ= -5.7666 ZZ= 58.2383
Eigenvalues: -42.1944 57.9615 153.6371
2 C Isotropic = 46.3050 Anisotropy = 114.9470
XX= 46.2821 YX= 1.1554 ZX= -31.2973
XY= 1.0543 YY= 122.3674 ZY= -8.3494
XZ= -35.0029 YZ= -8.1865 ZZ= -29.7347
Eigenvalues: -42.4884 58.4670 122.9363
3 C Isotropic = 70.3211 Anisotropy = 124.5086
XX= 48.6680 YX= 6.5228 ZX= 34.9287
XY= 6.3376 YY= 152.4192 ZY= -10.3985
XZ= 30.4046 YZ= -10.1437 ZZ= 9.8759
Eigenvalues: -9.6237 67.2600 153.3268
4 C Isotropic = 47.4347 Anisotropy = 140.0350
XX= -30.0329 YX= 6.8286 ZX= -2.8152
XY= 7.0687 YY= 140.0905 ZY= -6.7723
XZ= -1.4730 YZ= -6.5272 ZZ= 32.2466
Eigenvalues: -30.3724 31.8852 140.7914
5 C Isotropic = 58.7333 Anisotropy = 161.7694
XX= 20.9935 YX= 5.7564 ZX= -6.1364
XY= 5.3999 YY= 165.7344 ZY= -10.3116
XZ= -7.6062 YZ= -10.2939 ZZ= -10.5279
Eigenvalues: -12.4142 22.0345 166.5796
6 C Isotropic = 58.0816 Anisotropy = 171.8942
XX= -0.7620 YX= 9.4113 ZX= 34.7293
XY= 9.4890 YY= 171.5719 ZY= -11.6073
XZ= 39.3453 YZ= -11.9560 ZZ= 3.4349
Eigenvalues: -36.8345 38.4015 172.6777
7 N Isotropic = 112.4180 Anisotropy = 88.0135
XX= 67.3389 YX= 6.8860 ZX= 41.5757
XY= 6.5947 YY= 170.4503 ZY= -6.0640
XZ= 35.8674 YZ= -5.8225 ZZ= 99.4647
Eigenvalues: 40.8686 125.2917 171.0936
8 C Isotropic = 59.0253 Anisotropy = 122.1983
XX= 28.4575 YX= 3.4359 ZX= -19.7706
XY= 3.6473 YY= 139.9044 ZY= -7.2755
XZ= -31.4984 YZ= -6.5615 ZZ= 8.7139
Eigenvalues: -8.9764 45.5614 140.4908
9 C Isotropic = 75.6456 Anisotropy = 108.2643
XX= 58.2873 YX= 2.7171 ZX= -16.6856
XY= 2.5850 YY= 147.3095 ZY= -6.8642
XZ= -8.7219 YZ= -7.0921 ZZ= 21.3400
Eigenvalues: 17.1272 61.9878 147.8218
10 C Isotropic = 15.3468 Anisotropy = 119.2651
XX= -30.1640 YX= 7.7425 ZX= 45.5606
XY= 6.7911 YY= 94.0861 ZY= -8.4993
XZ= 25.8489 YZ= -7.6051 ZZ= -17.8818
Eigenvalues: -60.9966 12.1801 94.8569
11 Br Isotropic = 1894.0600 Anisotropy = 1569.9148
XX= 1661.7173 YX= 21.9920 ZX= 554.3591
XY= 18.3185 YY= 1331.3247 ZY= 53.5545
XZ= 573.6241 YZ= 63.4688 ZZ= 2689.1380
Eigenvalues: 1328.6389 1412.8713 2940.6699
12 C Isotropic = 100.2687 Anisotropy = 40.7510
XX= 49.7775 YX= 3.6413 ZX= 8.0495

XY= 4.1650 YY= 125.1569 ZY= -0.8674
XZ= 13.8616 YZ= -0.6300 ZZ= 125.8717
Eigenvalues: 48.0273 125.3427 127.4361
13 C Isotropic = 27.3914 Anisotropy = 134.3361
XX= 26.5139 YX= 3.5317 ZX= -1.9683
XY= 5.5956 YY= 116.1662 ZY= -9.8993
XZ= 29.9739 YZ= -11.1919 ZZ= -60.5059
Eigenvalues: -63.3934 28.6188 116.9488
14 N Isotropic = -113.2263 Anisotropy = 245.8080
XX= -115.0103 YX= 5.3728 ZX= -27.5300
XY= 6.4088 YY= 49.4554 ZY= -16.0422
XZ= -8.3253 YZ= -18.2722 ZZ= -274.1239
Eigenvalues: -276.9438 -113.3807 50.6457
15 O Isotropic = -42.4338 Anisotropy = 266.5200
XX= -123.4879 YX= 11.1849 ZX= 10.4065
XY= 12.7103 YY= 133.8076 ZY= -15.8795
XZ= 0.0479 YZ= -15.7093 ZZ= -137.6212
Eigenvalues: -140.6344 -121.9133 135.2461
16 C Isotropic = 62.4543 Anisotropy = 101.9378
XX= 41.4302 YX= 2.0512 ZX= 25.8185
XY= 1.6733 YY= 130.0015 ZY= -7.0544
XZ= 16.9411 YZ= -6.6016 ZZ= 15.9312
Eigenvalues: 3.4164 53.5337 130.4128
17 N Isotropic = 96.5845 Anisotropy = 126.1287
XX= 14.9879 YX= -0.6056 ZX= -28.0654
XY= 0.0411 YY= 180.4881 ZY= -2.8245
XZ= -23.0513 YZ= -5.0048 ZZ= 94.2775
Eigenvalues: 7.4525 101.6307 180.6703
18 C Isotropic = 63.8392 Anisotropy = 119.5954
XX= 53.0302 YX= 1.8689 ZX= 19.7142
XY= 1.5159 YY= 143.0309 ZY= -8.7182
XZ= 28.0142 YZ= -9.1308 ZZ= -4.5436
Eigenvalues: -13.6625 61.6106 143.5694
19 C Isotropic = 72.8971 Anisotropy = 133.0624
XX= 51.3535 YX= -0.4571 ZX= -23.2269
XY= -1.2240 YY= 161.0519 ZY= -9.3630
XZ= -27.2220 YZ= -9.1105 ZZ= 6.2857
Eigenvalues: -5.4669 62.5527 161.6053
20 C Isotropic = 69.9970 Anisotropy = 144.4655
XX= -3.0579 YX= 1.7968 ZX= 8.3074
XY= 2.0722 YY= 165.9381 ZY= -6.0041
XZ= 9.9968 YZ= -7.0426 ZZ= 47.1108
Eigenvalues: -4.7297 48.4134 166.3073
21 I Isotropic = 3879.6308 Anisotropy = 1460.5259
XX= 4821.8636 YX= -37.3435 ZX= 260.3130
XY= -58.5981 YY= 3723.0245 ZY= -49.0140
XZ= 190.6983 YZ= -39.1338 ZZ= 3094.0044
Eigenvalues: 3062.9105 3722.6673 4853.3147
22 H Isotropic = 24.0478 Anisotropy = 10.0414
XX= 23.4789 YX= -0.2798 ZX= -0.8103
XY= -0.3031 YY= 18.1168 ZY= 0.7903
XZ= -1.1920 YZ= 0.8169 ZZ= 30.5476
Eigenvalues: 18.0555 23.3458 30.7421
23 H Isotropic = 24.1023 Anisotropy = 10.4491
XX= 28.8203 YX= -0.2715 ZX= 3.0343
XY= -0.2412 YY= 17.5318 ZY= 0.4065
XZ= 3.7468 YZ= 0.3568 ZZ= 25.9549
Eigenvalues: 17.4978 23.7408 31.0684

24 H Isotropic = 22.8705 Anisotropy = 10.7002
XX= 25.5184 YX= -0.2192 ZX= 3.1246
XY= -0.2148 YY= 15.6343 ZY= 0.5753
XZ= 3.6183 YZ= 0.5490 ZZ= 27.4589
Eigenvalues: 15.5919 23.0158 30.0040
25 H Isotropic = 23.7908 Anisotropy = 8.9880
XX= 27.7445 YX= -0.6240 ZX= -2.0434
XY= -0.6436 YY= 15.3890 ZY= 0.8936
XZ= -1.3440 YZ= 0.8367 ZZ= 28.2389
Eigenvalues: 15.3090 26.2807 29.7828
26 H Isotropic = 22.8609 Anisotropy = 15.4670
XX= 21.7417 YX= -0.2786 ZX= 1.4077
XY= -0.4240 YY= 13.7368 ZY= 1.1080
XZ= -1.3596 YZ= 1.1928 ZZ= 33.1042
Eigenvalues: 13.6534 21.7570 33.1723
27 H Isotropic = 22.6592 Anisotropy = 8.1273
XX= 27.6203 YX= -0.1411 ZX= 0.7960
XY= 0.0525 YY= 14.4814 ZY= 0.5354
XZ= 1.2021 YZ= 0.6523 ZZ= 25.8758
Eigenvalues: 14.4499 25.4503 28.0774
28 H Isotropic = 24.6496 Anisotropy = 3.5545
XX= 26.0530 YX= -0.1277 ZX= -1.2070
XY= -0.0733 YY= 21.2063 ZY= 0.3759
XZ= 0.1294 YZ= 0.3362 ZZ= 26.6897
Eigenvalues: 21.1823 25.7472 27.0193
29 H Isotropic = 25.1561 Anisotropy = 3.2954
XX= 26.1163 YX= -0.0890 ZX= -0.7029
XY= -0.0834 YY= 22.1946 ZY= 0.3025
XZ= -0.2207 YZ= 0.3231 ZZ= 27.1575
Eigenvalues: 22.1741 25.9412 27.3530
30 H Isotropic = 23.7900 Anisotropy = 14.0438
XX= 22.3034 YX= -0.3720 ZX= -2.5351
XY= -0.2709 YY= 16.5827 ZY= 1.3369
XZ= -2.3574 YZ= 1.3035 ZZ= 32.4839
Eigenvalues: 16.4712 21.7462 33.1526

Isomer 5 (conformer 2)

1 C Isotropic = 58.2350 Anisotropy = 144.6445
XX= -26.7606 YX= 46.2242 ZX= -2.6005
XY= 46.9579 YY= 140.5741 ZY= 14.7647
XZ= 1.2334 YZ= 13.8237 ZZ= 60.8916
Eigenvalues: -39.0412 59.0816 154.6647
2 C Isotropic = 47.1173 Anisotropy = 114.0147
XX= 55.0996 YX= 20.1649 ZX= -21.9665
XY= 21.9182 YY= 112.7318 ZY= 32.1197
XZ= -26.3382 YZ= 29.6479 ZZ= -26.4795
Eigenvalues: -41.2811 59.5060 123.1271
3 C Isotropic = 70.1107 Anisotropy = 125.4076
XX= 48.5506 YX= 18.0395 ZX= 39.8035
XY= 17.0292 YY= 147.3699 ZY= 14.8951
XZ= 33.5600 YZ= 14.4879 ZZ= 14.4115
Eigenvalues: -9.0362 65.6525 153.7157
4 C Isotropic = 47.1073 Anisotropy = 140.8919
XX= -22.3960 YX= 34.6600 ZX= -0.6935
XY= 36.9933 YY= 130.0088 ZY= 19.8765
XZ= 0.0605 YZ= 17.1681 ZZ= 33.7090
Eigenvalues: -30.7001 30.9867 141.0352
5 C Isotropic = 58.9151 Anisotropy = 164.4865
XX= 25.8291 YX= 35.6454 ZX= 1.0912
XY= 32.4003 YY= 156.7464 ZY= 24.7660
XZ= -1.6949 YZ= 26.3000 ZZ= -5.8302
Eigenvalues: -10.7385 18.9110 168.5728
6 C Isotropic = 58.4189 Anisotropy = 174.3631
XX= 2.7371 YX= 39.2921 ZX= 38.2940
XY= 35.1269 YY= 164.5901 ZY= 7.4929
XZ= 41.8744 YZ= 10.7960 ZZ= 7.9295
Eigenvalues: -37.1418 37.7375 174.6610
7 N Isotropic = 113.0387 Anisotropy = 90.3384
XX= 67.8133 YX= 17.3686 ZX= 41.8094
XY= 23.2004 YY= 167.4385 ZY= 3.2260
XZ= 31.3587 YZ= 3.5899 ZZ= 103.8644
Eigenvalues: 43.1070 122.7448 173.2643
8 C Isotropic = 59.0996 Anisotropy = 118.8516
XX= 41.5891 YX= 26.0849 ZX= -23.0637
XY= 25.6853 YY= 129.3668 ZY= 20.2110
XZ= -34.3896 YZ= 26.9125 ZZ= 6.3430
Eigenvalues: -17.3350 56.2999 138.3341
9 C Isotropic = 76.4673 Anisotropy = 105.1177
XX= 73.0929 YX= 16.9115 ZX= -12.8068
XY= 15.8704 YY= 141.2182 ZY= 14.8815
XZ= -5.4182 YZ= 18.6898 ZZ= 15.0907
Eigenvalues: 10.8373 72.0188 146.5457
10 C Isotropic = 14.1038 Anisotropy = 121.1774
XX= 37.5959 YX= -41.7493 ZX= -10.3378
XY= -34.3734 YY= 65.1350 ZY= -37.0605
XZ= 1.6286 YZ= -21.3570 ZZ= -60.4194
Eigenvalues: -68.4906 15.9133 94.8888
11 Br Isotropic = 1892.6799 Anisotropy = 1578.6932
XX= 1587.5157 YX= -140.1998 ZX= 457.5140
XY= -139.3066 YY= 1404.7692 ZY= -343.3600
XZ= 479.0600 YZ= -333.1047 ZZ= 2685.7548
Eigenvalues: 1316.0264 1416.8712 2945.1420
12 C Isotropic = 91.9441 Anisotropy = 47.3074
XX= 94.8140 YX= -28.3794 ZX= -29.6903

XY= -26.5274 YY= 96.9297 ZY= -28.5155
XZ= -33.1442 YZ= -33.9405 ZZ= 84.0887
Eigenvalues: 31.2604 121.0896 123.4824
13 C Isotropic = 26.2983 Anisotropy = 136.0775
XX= 42.8869 YX= -43.0724 ZX= 50.6271
XY= -52.6572 YY= 83.5281 ZY= 15.4223
XZ= 25.6298 YZ= -4.8788 ZZ= -47.5200
Eigenvalues: -64.8869 26.7652 117.0167
14 N Isotropic = -121.7287 Anisotropy = 258.7258
XX= -115.4139 YX= -97.7507 ZX= 96.0632
XY= -131.8624 YY= -36.0646 ZY= 19.0073
XZ= 82.8043 YZ= 24.0146 ZZ= -213.7076
Eigenvalues: -293.1047 -122.8366 50.7551
15 O Isotropic = -56.5839 Anisotropy = 267.1007
XX= -61.0311 YX= -120.3451 ZX= 30.4805
XY= -125.0769 YY= 31.4983 ZY= -40.1130
XZ= 24.7309 YZ= -10.5561 ZZ= -140.2191
Eigenvalues: -153.8349 -137.4001 121.4832
16 C Isotropic = 62.2035 Anisotropy = 102.1254
XX= 71.6778 YX= -33.4566 ZX= 4.0901
XY= -33.0520 YY= 110.6587 ZY= -8.2868
XZ= 11.6285 YZ= -2.2879 ZZ= 4.2739
Eigenvalues: 3.3465 52.9769 130.2871
17 N Isotropic = 97.1765 Anisotropy = 126.3546
XX= 60.0717 YX= -70.4373 ZX= -20.9915
XY= -74.4073 YY= 138.0132 ZY= -13.9737
XZ= -22.8107 YZ= -19.8267 ZZ= 93.4445
Eigenvalues: 7.9668 102.1497 181.4129
18 C Isotropic = 63.8532 Anisotropy = 119.5533
XX= 75.8720 YX= -36.4792 ZX= 24.4795
XY= -35.6181 YY= 123.5161 ZY= 2.5244
XZ= 17.6500 YZ= -2.1383 ZZ= -7.8287
Eigenvalues: -13.4164 61.4205 143.5554
19 C Isotropic = 72.6837 Anisotropy = 133.5454
XX= 46.4920 YX= -63.0905 ZX= 28.8324
XY= -61.3044 YY= 127.3847 ZY= 6.1017
XZ= 31.9970 YZ= 8.5519 ZZ= 44.1745
Eigenvalues: -5.7131 62.0503 161.7140
20 C Isotropic = 69.3065 Anisotropy = 145.8343
XX= 59.2501 YX= -62.9848 ZX= -19.1870
XY= -66.0259 YY= 127.1875 ZY= -18.7307
XZ= -18.3701 YZ= -21.6045 ZZ= 21.4819
Eigenvalues: -5.7693 47.1594 166.5294
21 I Isotropic = 3880.2533 Anisotropy = 1637.7240
XX= 4034.1419 YX= 471.5326 ZX= 542.8786
XY= 513.5265 YY= 4181.0492 ZY= 454.5954
XZ= 632.2375 YZ= 512.4581 ZZ= 3425.5688
Eigenvalues: 3037.6802 3631.0104 4972.0693
22 H Isotropic = 24.1217 Anisotropy = 10.6474
XX= 22.8706 YX= -0.9741 ZX= -1.2433
XY= -1.2855 YY= 18.9899 ZY= -2.7644
XZ= -1.8381 YZ= -2.2157 ZZ= 30.5046
Eigenvalues: 18.0461 23.0990 31.2200
23 H Isotropic = 24.0937 Anisotropy = 9.7247
XX= 27.8188 YX= -2.5062 ZX= 2.3816
XY= -2.5917 YY= 18.5739 ZY= -2.0799
XZ= 2.8915 YZ= -2.1934 ZZ= 25.8884
Eigenvalues: 17.6470 24.0574 30.5768

 24 H Isotropic = 23.5881 Anisotropy = 11.7840
XX= 22.7286 YX= -1.4588 ZX= 2.5791
XY= -2.3198 YY= 21.9154 ZY= -6.8554
XZ= 1.8479 YZ= -5.3641 ZZ= 26.1202
Eigenvalues: 17.5424 21.7777 31.4441
 25 H Isotropic = 23.7852 Anisotropy = 9.9273
XX= 28.2380 YX= -1.7169 ZX= -3.0596
XY= -1.5165 YY= 16.1789 ZY= -1.2286
XZ= -2.3847 YZ= -1.3475 ZZ= 26.9386
Eigenvalues: 15.7172 25.2349 30.4034
 26 H Isotropic = 24.0988 Anisotropy = 5.9854
XX= 27.1016 YX= -0.4168 ZX= -0.8727
XY= -1.7112 YY= 19.4012 ZY= -0.0745
XZ= -1.9907 YZ= -0.4371 ZZ= 25.7934
Eigenvalues: 19.2255 24.9817 28.0891
 27 H Isotropic = 22.7088 Anisotropy = 7.9351
XX= 24.6770 YX= 5.6130 ZX= 0.6089
XY= 5.5280 YY= 17.9840 ZY= 0.7475
XZ= -0.0297 YZ= 0.8806 ZZ= 25.4653
Eigenvalues: 14.8020 25.3255 27.9988
 28 H Isotropic = 24.6663 Anisotropy = 3.5809
XX= 24.6283 YX= 1.8396 ZX= 0.3125
XY= 1.8387 YY= 22.3510 ZY= 0.6629
XZ= -0.8339 YZ= 0.0129 ZZ= 27.0196
Eigenvalues: 21.2954 25.6499 27.0535
 29 H Isotropic = 25.1411 Anisotropy = 3.3692
XX= 25.0387 YX= 1.5134 ZX= -0.3038
XY= 1.5970 YY= 23.0996 ZY= 0.2486
XZ= -0.6478 YZ= 0.1055 ZZ= 27.2849
Eigenvalues: 22.2070 25.8290 27.3872
 30 H Isotropic = 23.7515 Anisotropy = 13.8266
XX= 22.1935 YX= 2.2987 ZX= -4.3412
XY= 2.3447 YY= 17.8772 ZY= -0.3988
XZ= -4.2363 YZ= 0.1074 ZZ= 31.1839
Eigenvalues: 16.6591 21.6262 32.9692

Isomer 5 (conformer 3)

1 C Isotropic = 56.3539 Anisotropy = 146.2137
XX= -42.3167 YX= -0.9838 ZX= 0.5535
XY= -1.4231 YY= 153.7467 ZY= -2.6304
XZ= 2.9528 YZ= -2.7413 ZZ= 57.6317
Eigenvalues: -42.3543 57.5863 153.8297
2 C Isotropic = 46.0911 Anisotropy = 115.6868
XX= 42.6483 YX= -1.4769 ZX= -33.8206
XY= -1.7721 YY= 123.0537 ZY= -5.0509
XZ= -37.8713 YZ= -4.7402 ZZ= -27.4285
Eigenvalues: -42.6757 57.7335 123.2157
3 C Isotropic = 70.3197 Anisotropy = 124.8086
XX= 50.9839 YX= 0.5340 ZX= 33.6769
XY= 0.6428 YY= 153.3975 ZY= -4.4679
XZ= 29.1412 YZ= -4.1644 ZZ= 6.5777
Eigenvalues: -9.7868 67.2205 153.5254
4 C Isotropic = 47.2533 Anisotropy = 139.9383
XX= -30.6775 YX= -0.4441 ZX= 0.3003
XY= -0.5604 YY= 140.4580 ZY= -3.0619
XZ= 1.6878 YZ= -3.0453 ZZ= 31.9796
Eigenvalues: -30.6945 31.9090 140.5455
5 C Isotropic = 58.8620 Anisotropy = 161.7933
XX= 20.3964 YX= -0.7810 ZX= -7.1359
XY= -0.0243 YY= 166.5853 ZY= -5.0164
XZ= -8.7297 YZ= -4.8940 ZZ= -10.3958
Eigenvalues: -12.4540 22.3157 166.7242
6 C Isotropic = 57.9294 Anisotropy = 172.7576
XX= 1.4596 YX= 0.2212 ZX= 35.0102
XY= 1.0964 YY= 172.9966 ZY= -3.7340
XZ= 39.6478 YZ= -4.7748 ZZ= -0.6680
Eigenvalues: -37.0070 37.6941 173.1011
7 N Isotropic = 112.5752 Anisotropy = 87.8332
XX= 71.0453 YX= 0.8554 ZX= 43.2506
XY= 0.2474 YY= 171.0635 ZY= -2.2388
XZ= 37.4738 YZ= -2.1051 ZZ= 95.6169
Eigenvalues: 41.1172 125.4777 171.1307
8 C Isotropic = 60.0441 Anisotropy = 120.8647
XX= 26.6985 YX= -0.8875 ZX= -20.1641
XY= -0.2967 YY= 140.4412 ZY= -5.7263
XZ= -32.4181 YZ= -3.8050 ZZ= 12.9926
Eigenvalues: -7.4397 46.9514 140.6205
9 C Isotropic = 75.4226 Anisotropy = 108.2403
XX= 56.7556 YX= -0.6544 ZX= -17.9612
XY= -0.3069 YY= 147.4936 ZY= -2.9765
XZ= -9.8471 YZ= -3.7130 ZZ= 22.0185
Eigenvalues: 17.0544 61.6305 147.5828
10 C Isotropic = 15.3226 Anisotropy = 120.4529
XX= -25.4707 YX= 6.8386 ZX= 44.8935
XY= 5.1203 YY= 95.2812 ZY= -4.6189
XZ= 24.9240 YZ= -3.4131 ZZ= -23.8427
Eigenvalues: -59.8983 10.2416 95.6245
11 Br Isotropic = 1891.6161 Anisotropy = 1574.8139
XX= 1709.8824 YX= 20.7026 ZX= 598.5304
XY= 18.7279 YY= 1325.4750 ZY= 40.9650
XZ= 617.8576 YZ= 43.2215 ZZ= 2639.4908
Eigenvalues: 1324.1273 1409.2288 2941.4920
12 C Isotropic = 104.7817 Anisotropy = 50.0496
XX= 53.4824 YX= 3.9744 ZX= 11.1808

XY= 2.8520 YY= 125.2494 ZY= 2.7805
XZ= 16.8317 YZ= -0.5756 ZZ= 135.6133
Eigenvalues: 51.0227 125.1743 138.1481
13 C Isotropic = 28.2496 Anisotropy = 133.6186
XX= 28.5850 YX= 4.1247 ZX= -3.1772
XY= 4.8479 YY= 117.0559 ZY= -2.5478
XZ= 26.6110 YZ= -4.3437 ZZ= -60.8919
Eigenvalues: -62.4895 29.9097 117.3287
14 N Isotropic = -126.2430 Anisotropy = 257.1768
XX= -122.5381 YX= 6.8014 ZX= -30.9534
XY= 8.4885 YY= 44.7158 ZY= -6.0720
XZ= -19.4255 YZ= -5.6746 ZZ= -300.9068
Eigenvalues: -304.4610 -119.4762 45.2082
15 O Isotropic = -48.3414 Anisotropy = 279.7114
XX= -132.2610 YX= 11.9971 ZX= 11.9678
XY= 9.5263 YY= 137.6107 ZY= -5.7635
XZ= -5.2643 YZ= -4.9120 ZZ= -150.3739
Eigenvalues: -151.1543 -132.0028 138.1329
16 C Isotropic = 61.8902 Anisotropy = 98.5355
XX= 37.4686 YX= 6.0393 ZX= -35.0841
XY= 6.1158 YY= 127.1341 ZY= 0.5764
XZ= -29.6613 YZ= 0.0704 ZZ= 21.0677
Eigenvalues: -4.2483 62.3383 127.5805
17 N Isotropic = 93.4051 Anisotropy = 141.1206
XX= 10.2582 YX= 13.0671 ZX= 15.9366
XY= 12.6511 YY= 186.4922 ZY= -4.0049
XZ= 17.6212 YZ= -3.3984 ZZ= 83.4649
Eigenvalues: 5.6100 87.1199 187.4855
18 C Isotropic = 65.5146 Anisotropy = 114.8975
XX= 51.1679 YX= 6.1800 ZX= -24.3873
XY= 6.4431 YY= 141.6330 ZY= -0.5211
XZ= -35.2217 YZ= 0.0117 ZZ= 3.7430
Eigenvalues: -10.6727 65.1036 142.1130
19 C Isotropic = 72.1481 Anisotropy = 138.0788
XX= 51.7412 YX= 8.4944 ZX= 20.0097
XY= 8.7510 YY= 163.4837 ZY= -4.5706
XZ= 22.4143 YZ= -4.6390 ZZ= 1.2194
Eigenvalues: -6.8176 59.0613 164.2006
20 C Isotropic = 70.2980 Anisotropy = 139.6367
XX= -1.2341 YX= 11.7192 ZX= -13.9828
XY= 11.6760 YY= 162.5019 ZY= -1.9352
XZ= -11.7961 YZ= -1.2587 ZZ= 49.6262
Eigenvalues: -5.0386 52.5435 163.3891
21 I Isotropic = 3902.7654 Anisotropy = 1465.0050
XX= 4859.7187 YX= -61.6855 ZX= 191.3424
XY= -93.6725 YY= 3749.9964 ZY= -33.3768
XZ= 126.1248 YZ= -2.9084 ZZ= 3098.5810
Eigenvalues: 3084.2007 3744.6600 4879.4354
22 H Isotropic = 24.0399 Anisotropy = 10.0404
XX= 23.3939 YX= -0.0277 ZX= -0.5324
XY= 0.0020 YY= 18.0731 ZY= 0.3867
XZ= -0.8994 YZ= 0.3563 ZZ= 30.6527
Eigenvalues: 18.0621 23.3241 30.7335
23 H Isotropic = 24.1094 Anisotropy = 10.4584
XX= 29.1061 YX= 0.1141 ZX= 2.9007
XY= 0.1285 YY= 17.5441 ZY= 0.2384
XZ= 3.6255 YZ= 0.2309 ZZ= 25.6778
Eigenvalues: 17.5373 23.7091 31.0816

 24 H Isotropic = 22.8288 Anisotropy = 10.6271
XX= 25.8044 YX= 0.0380 ZX= 3.1658
XY= 0.0856 YY= 15.5825 ZY= 0.5145
XZ= 3.6148 YZ= 0.3663 ZZ= 27.0995
Eigenvalues: 15.5652 23.0077 29.9136
 25 H Isotropic = 23.8137 Anisotropy = 8.9618
XX= 27.6348 YX= -0.0530 ZX= -2.0487
XY= -0.0922 YY= 15.3545 ZY= 0.2826
XZ= -1.3333 YZ= 0.3086 ZZ= 28.4517
Eigenvalues: 15.3477 26.3051 29.7882
 26 H Isotropic = 23.0785 Anisotropy = 15.2666
XX= 21.9678 YX= -0.0762 ZX= 1.7549
XY= -0.0177 YY= 14.0261 ZY= 0.0078
XZ= -0.9444 YZ= -0.0318 ZZ= 33.2417
Eigenvalues: 14.0258 21.9535 33.2563
 27 H Isotropic = 21.5057 Anisotropy = 20.9076
XX= 23.1753 YX= -0.9744 ZX= -6.0743
XY= -1.0510 YY= 8.5480 ZY= 0.5186
XZ= -5.2543 YZ= 0.4937 ZZ= 32.7936
Eigenvalues: 8.4777 20.5952 35.4441
 28 H Isotropic = 24.6926 Anisotropy = 4.3582
XX= 25.5454 YX= -0.3018 ZX= 0.4493
XY= -0.2854 YY= 20.9511 ZY= 0.0697
XZ= -0.7880 YZ= 0.1589 ZZ= 27.5812
Eigenvalues: 20.9308 25.5488 27.5980
 29 H Isotropic = 25.1053 Anisotropy = 2.5938
XX= 26.2454 YX= -0.2568 ZX= -0.0106
XY= -0.2572 YY= 22.3627 ZY= 0.0479
XZ= -0.5164 YZ= 0.1147 ZZ= 26.7079
Eigenvalues: 22.3448 26.1366 26.8345
 30 H Isotropic = 24.1713 Anisotropy = 4.9234
XX= 25.2270 YX= -0.3265 ZX= -0.9182
XY= -0.4050 YY= 20.0223 ZY= 0.2964
XZ= -0.3254 YZ= 0.1704 ZZ= 27.2646
Eigenvalues: 19.9917 25.0687 27.4536

Isomer 5 (conformer 4)

1 C Isotropic = 58.1308 Anisotropy = 144.7861
XX= -20.4765 YX= 55.6502 ZX= -5.9121
XY= 56.9678 YY= 135.5866 ZY= 11.6008
XZ= -2.0633 YZ= 10.1272 ZZ= 59.2825
Eigenvalues: -39.1911 58.9288 154.6549
2 C Isotropic = 46.9559 Anisotropy = 114.2061
XX= 58.2340 YX= 22.0946 ZX= -19.8387
XY= 23.8138 YY= 112.8961 ZY= 26.4116
XZ= -24.4935 YZ= 24.0504 ZZ= -30.2623
Eigenvalues: -41.3735 59.1479 123.0933
3 C Isotropic = 69.8076 Anisotropy = 126.0100
XX= 49.2641 YX= 26.0478 ZX= 39.8199
XY= 24.3073 YY= 146.0332 ZY= 5.9949
XZ= 33.4305 YZ= 5.8890 ZZ= 14.1254
Eigenvalues: -9.4010 65.0095 153.8142
4 C Isotropic = 46.9887 Anisotropy = 140.6894
XX= -17.7335 YX= 43.1503 ZX= -2.4870
XY= 44.9377 YY= 126.9735 ZY= 15.0697
XZ= -2.0262 YZ= 12.3531 ZZ= 31.7261
Eigenvalues: -30.6466 30.8311 140.7816
5 C Isotropic = 59.0295 Anisotropy = 164.9638
XX= 30.2126 YX= 43.3351 ZX= 0.5388
XY= 39.8900 YY= 155.0649 ZY= 15.1976
XZ= -2.1432 YZ= 17.4984 ZZ= -8.1892
Eigenvalues: -10.5962 18.6792 169.0053
6 C Isotropic = 59.0649 Anisotropy = 173.4855
XX= 8.3416 YX= 50.7266 ZX= 35.9036
XY= 47.4802 YY= 159.7010 ZY= -4.1866
XZ= 40.3271 YZ= -0.0902 ZZ= 9.1522
Eigenvalues: -36.6048 39.0777 174.7220
7 N Isotropic = 112.8106 Anisotropy = 91.3514
XX= 69.0305 YX= 25.8666 ZX= 40.1764
XY= 30.6198 YY= 165.0314 ZY= -1.6787
XZ= 29.4555 YZ= -1.4588 ZZ= 104.3698
Eigenvalues: 42.5094 122.2108 173.7115
8 C Isotropic = 58.8360 Anisotropy = 119.1923
XX= 45.4050 YX= 29.5433 ZX= -23.1077
XY= 28.1617 YY= 128.6199 ZY= 14.7139
XZ= -33.6674 YZ= 22.0022 ZZ= 2.4830
Eigenvalues: -17.6733 55.8837 138.2975
9 C Isotropic = 76.6723 Anisotropy = 104.9109
XX= 76.0346 YX= 19.5532 ZX= -12.4940
XY= 19.7091 YY= 140.6923 ZY= 8.0740
XZ= -4.6355 YZ= 12.2955 ZZ= 13.2899
Eigenvalues: 10.8500 72.5541 146.6129
10 C Isotropic = 14.3823 Anisotropy = 122.0103
XX= 34.5841 YX= -41.3501 ZX= -6.3956
XY= -32.0697 YY= 65.8701 ZY= -41.4067
XZ= 6.7498 YZ= -27.5247 ZZ= -57.3072
Eigenvalues: -67.1852 14.6097 95.7225
11 Br Isotropic = 1889.5416 Anisotropy = 1584.7678
XX= 1555.4075 YX= -124.4128 ZX= 432.9667
XY= -118.4845 YY= 1379.6776 ZY= -296.3816
XZ= 451.3107 YZ= -295.4928 ZZ= 2733.5397
Eigenvalues: 1310.0788 1412.4925 2946.0535
12 C Isotropic = 96.0925 Anisotropy = 53.1279
XX= 97.1825 YX= -28.2354 ZX= -35.3455

XY= -27.9089 YY= 97.4713 ZY= -26.2266
XZ= -36.7528 YZ= -33.9108 ZZ= 93.6238
Eigenvalues: 33.0462 123.7203 131.5111
13 C Isotropic = 27.5521 Anisotropy = 134.8191
XX= 40.2580 YX= -37.9548 ZX= 52.5873
XY= -48.3185 YY= 87.8971 ZY= 4.7545
XZ= 29.9852 YZ= -13.8731 ZZ= -45.4988
Eigenvalues: -63.1815 28.4063 117.4315
14 N Isotropic = -134.1493 Anisotropy = 270.9130
XX= -141.1385 YX= -93.5734 ZX= 112.0278
XY= -121.8686 YY= -29.2909 ZY= 0.4563
XZ= 104.4953 YZ= 14.3029 ZZ= -232.0184
Eigenvalues: -320.5029 -128.4043 46.4593
15 O Isotropic = -62.9461 Anisotropy = 279.8805
XX= -82.7672 YX= -124.4113 ZX= 33.4400
XY= -117.8929 YY= 40.4701 ZY= -49.8058
XZ= 36.7687 YZ= -21.8813 ZZ= -146.5413
Eigenvalues: -167.2781 -145.2011 123.6409
16 C Isotropic = 61.8194 Anisotropy = 99.2207
XX= 39.5878 YX= -54.3300 ZX= 28.8099
XY= -55.6745 YY= 89.6867 ZY= 1.8182
XZ= 24.5400 YZ= -0.7454 ZZ= 56.1838
Eigenvalues: -4.5227 62.0145 127.9665
17 N Isotropic = 92.6787 Anisotropy = 143.0131
XX= 95.1769 YX= -68.7469 ZX= -17.2910
XY= -69.8572 YY= 128.9487 ZY= -43.4286
XZ= -17.9361 YZ= -44.8394 ZZ= 53.9105
Eigenvalues: 4.3185 85.6967 188.0207
18 C Isotropic = 65.1407 Anisotropy = 115.6292
XX= 47.7861 YX= -57.2255 ZX= 34.7304
XY= -57.0116 YY= 102.8695 ZY= 0.8155
XZ= 43.7096 YZ= 7.0996 ZZ= 44.7666
Eigenvalues: -11.2119 64.4072 142.2269
19 C Isotropic = 72.0227 Anisotropy = 137.9710
XX= 87.5796 YX= -46.2782 ZX= 28.4991
XY= -46.6476 YY= 126.9375 ZY= -19.7118
XZ= 26.2850 YZ= -20.3557 ZZ= 1.5510
Eigenvalues: -6.7869 58.8516 164.0034
20 C Isotropic = 70.6785 Anisotropy = 139.9563
XX= 54.3340 YX= -76.0158 ZX= 1.1850
XY= -74.6559 YY= 105.2367 ZY= -28.1435
XZ= -1.7799 YZ= -28.0858 ZZ= 52.4648
Eigenvalues: -4.8411 52.8938 163.9827
21 I Isotropic = 3906.2577 Anisotropy = 1601.9022
XX= 4085.1490 YX= 505.9012 ZX= 559.6843
XY= 494.5723 YY= 4202.2663 ZY= 377.7424
XZ= 636.4444 YZ= 445.0612 ZZ= 3431.3578
Eigenvalues: 3065.0735 3679.5071 4974.1925
22 H Isotropic = 24.1385 Anisotropy = 10.6214
XX= 22.7686 YX= -1.2516 ZX= -1.4054
XY= -1.6414 YY= 18.9405 ZY= -2.0698
XZ= -1.9548 YZ= -1.4395 ZZ= 30.7066
Eigenvalues: 18.0669 23.1293 31.2195
23 H Isotropic = 24.0870 Anisotropy = 9.7256
XX= 27.3993 YX= -2.8941 ZX= 2.3992
XY= -2.9392 YY= 18.6911 ZY= -1.9320
XZ= 2.9718 YZ= -1.9725 ZZ= 26.1707
Eigenvalues: 17.6490 24.0413 30.5707

 24 H Isotropic = 23.7431 Anisotropy = 11.5941
XX= 22.6557 YX= -1.4493 ZX= 2.2284
XY= -2.2157 YY= 21.6602 ZY= -6.6068
XZ= 1.7358 YZ= -5.0267 ZZ= 26.9134
Eigenvalues: 17.8538 21.9030 31.4725
 25 H Isotropic = 23.7511 Anisotropy = 9.8611
XX= 27.9835 YX= -2.6031 ZX= -2.9782
XY= -2.3406 YY= 16.3439 ZY= -0.4706
XZ= -2.2889 YZ= -0.6281 ZZ= 26.9259
Eigenvalues: 15.7351 25.1930 30.3252
 26 H Isotropic = 24.1076 Anisotropy = 5.9701
XX= 27.0167 YX= -0.8958 ZX= -0.8203
XY= -2.2871 YY= 19.6080 ZY= 0.2144
XZ= -1.8537 YZ= 0.0098 ZZ= 25.6982
Eigenvalues: 19.2765 24.9587 28.0877
 27 H Isotropic = 21.4517 Anisotropy = 20.9140
XX= 17.1604 YX= 5.0167 ZX= -3.5181
XY= 5.3341 YY= 12.7397 ZY= 2.9603
XZ= -3.9959 YZ= 2.9128 ZZ= 34.4552
Eigenvalues: 8.5283 20.4325 35.3944
 28 H Isotropic = 24.6738 Anisotropy = 4.4026
XX= 24.5373 YX= 2.0084 ZX= -1.7744
XY= 2.1867 YY= 22.4308 ZY= 0.0298
XZ= -0.7251 YZ= 0.8373 ZZ= 27.0534
Eigenvalues: 20.9603 25.4523 27.6089
 29 H Isotropic = 25.1329 Anisotropy = 2.5856
XX= 25.0321 YX= 1.5473 ZX= -0.6375
XY= 1.6728 YY= 23.6415 ZY= 0.4263
XZ= -0.2529 YZ= 0.7654 ZZ= 26.7251
Eigenvalues: 22.4540 26.0881 26.8566
 30 H Isotropic = 24.1909 Anisotropy = 4.7395
XX= 23.8008 YX= 1.9818 ZX= -0.8604
XY= 2.0196 YY= 21.7667 ZY= 1.1788
XZ= -1.3022 YZ= 0.5721 ZZ= 27.0054
Eigenvalues: 20.2817 24.9405 27.3506

Isomer 6 (conformer 1)

1 C Isotropic = 57.2696 Anisotropy = 144.1232
XX= 51.2138 YX= 13.7178 ZX= 31.4704
XY= 13.3677 YY= 149.1287 ZY= 16.0790
XZ= 33.7598 YZ= 16.0752 ZZ= -28.5337
Eigenvalues: -40.7742 59.2312 153.3517
2 C Isotropic = 46.9545 Anisotropy = 112.9178
XX= -37.2473 YX= 25.6251 ZX= 9.7885
XY= 26.9290 YY= 117.0491 ZY= 5.3769
XZ= 6.1204 YZ= 6.4128 ZZ= 61.0615
Eigenvalues: -42.0606 60.6909 122.2330
3 C Isotropic = 70.7946 Anisotropy = 123.5821
XX= 36.5097 YX= 24.0444 ZX= -33.1236
XY= 24.3391 YY= 146.5292 ZY= 20.4019
XZ= -37.3768 YZ= 21.4440 ZZ= 29.3450
Eigenvalues: -8.9917 68.1929 153.1827
4 C Isotropic = 47.0799 Anisotropy = 141.8484
XX= 26.9586 YX= 17.2718 ZX= 21.0192
XY= 16.6968 YY= 136.8435 ZY= 15.8536
XZ= 22.2412 YZ= 16.0120 ZZ= -22.5622
Eigenvalues: -31.1768 30.7711 141.6456
5 C Isotropic = 58.0845 Anisotropy = 162.9018
XX= -6.7179 YX= 30.1820 ZX= -0.6771
XY= 30.2876 YY= 159.0794 ZY= 19.4341
XZ= -2.4256 YZ= 17.8754 ZZ= 21.8919
Eigenvalues: -12.7541 20.3219 166.6857
6 C Isotropic = 56.3390 Anisotropy = 174.6488
XX= 25.1825 YX= 28.5661 ZX= -26.3662
XY= 26.3797 YY= 164.7021 ZY= 29.1863
XZ= -22.4449 YZ= 27.2437 ZZ= -20.8677
Eigenvalues: -38.1562 34.4016 172.7715
7 N Isotropic = 114.9693 Anisotropy = 83.6796
XX= 124.4054 YX= 10.2001 ZX= -16.9522
XY= 11.2352 YY= 166.9120 ZY= 15.7112
XZ= -23.9150 YZ= 18.0431 ZZ= 53.5904
Eigenvalues: 45.1193 129.0329 170.7556
8 C Isotropic = 58.9320 Anisotropy = 123.4866
XX= -2.5807 YX= 22.3492 ZX= 25.6102
XY= 25.2575 YY= 135.8851 ZY= 7.4385
XZ= 12.3535 YZ= 9.6395 ZZ= 43.4917
Eigenvalues: -12.0436 47.5833 141.2564
9 C Isotropic = 75.1203 Anisotropy = 110.1574
XX= 19.3422 YX= 23.9365 ZX= -6.1147
XY= 22.1027 YY= 143.0605 ZY= 12.2256
XZ= 1.8226 YZ= 10.4069 ZZ= 62.9582
Eigenvalues: 14.8391 61.9632 148.5585
10 C Isotropic = 23.5095 Anisotropy = 133.7380
XX= -49.5200 YX= 27.0695 ZX= -9.3530
XY= 33.0173 YY= 104.5472 ZY= 17.1835
XZ= -39.5206 YZ= 22.7844 ZZ= 15.5013
Eigenvalues: -64.8812 22.7416 112.6682
11 Br Isotropic = 1907.8323 Anisotropy = 1566.0076
XX= 2890.8508 YX= -234.8794 ZX= -196.4375
XY= -246.8226 YY= 1376.6187 ZY= 18.1739

XZ= -178.5464 YZ= 15.8394 ZZ= 1456.0275
Eigenvalues: 1337.7454 1433.9143 2951.8374
12 C Isotropic = 100.9029 Anisotropy = 39.7278
XX= 99.7223 YX= -3.1498 ZX= 40.8234
XY= -2.9193 YY= 125.8233 ZY= 0.7037
XZ= 31.6684 YZ= 3.5746 ZZ= 77.1630
Eigenvalues: 50.3179 125.0027 127.3881
13 C Isotropic = 20.7308 Anisotropy = 121.4629
XX= -47.3749 YX= 21.9306 ZX= 13.6010
XY= 17.4426 YY= 96.5882 ZY= 13.2034
XZ= 34.4797 YZ= 9.6822 ZZ= 12.9792
Eigenvalues: -57.2415 17.7279 101.7061
14 O Isotropic = -31.5018 Anisotropy = 246.6559
XX= -103.8351 YX= 38.5354 ZX= -4.0175
XY= 35.1432 YY= 119.7340 ZY= 44.1430
XZ= 12.7875 YZ= 39.7461 ZZ= -110.4043
Eigenvalues: -118.3016 -109.1392 132.9355
15 N Isotropic = -123.7620 Anisotropy = 254.6614
XX= -227.9521 YX= 56.9453 ZX= -74.0740
XY= 58.7758 YY= 28.1651 ZY= 48.6832
XZ= -91.0643 YZ= 52.0404 ZZ= -171.4988
Eigenvalues: -304.5263 -112.7718 46.0123
16 C Isotropic = 62.9349 Anisotropy = 100.9709
XX= 38.4369 YX= 17.5519 ZX= -15.8002
XY= 18.8039 YY= 123.1650 ZY= 21.7617
XZ= -24.1215 YZ= 23.2352 ZZ= 27.2029
Eigenvalues: 5.0091 53.5468 130.2488
17 N Isotropic = 97.2311 Anisotropy = 125.9963
XX= 78.8044 YX= 8.3905 ZX= 41.3118
XY= 8.0405 YY= 176.0576 ZY= 20.6204
XZ= 46.1347 YZ= 20.0024 ZZ= 36.8314
Eigenvalues: 8.3205 102.1442 181.2286
18 C Isotropic = 62.8064 Anisotropy = 120.7486
XX= 16.9809 YX= 26.4423 ZX= -34.0746
XY= 25.1989 YY= 134.4749 ZY= 25.6958
XZ= -27.3673 YZ= 24.3477 ZZ= 36.9635
Eigenvalues: -13.8930 59.0068 143.3055
19 C Isotropic = 71.4906 Anisotropy = 134.8672
XX= -2.0680 YX= 23.3228 ZX= 13.8729
XY= 24.0180 YY= 154.4997 ZY= 16.5345
XZ= 10.4138 YZ= 16.9427 ZZ= 62.0401
Eigenvalues: -6.9348 60.0046 161.4021
20 C Isotropic = 69.2876 Anisotropy = 143.8705
XX= 47.4418 YX= 16.3961 ZX= 12.5168
XY= 16.6575 YY= 157.2587 ZY= 28.2822
XZ= 11.6895 YZ= 28.4596 ZZ= 3.1622
Eigenvalues: -3.5552 46.2167 165.2012
21 I Isotropic = 3884.4938 Anisotropy = 1464.2134
XX= 3382.9709 YX= 172.2218 ZX= -676.0309
XY= 175.2429 YY= 3703.8166 ZY= -54.6166
XZ= -605.2804 YZ= -65.9318 ZZ= 4566.6939
Eigenvalues: 3073.3151 3719.5302 4860.6361
22 H Isotropic = 24.1101 Anisotropy = 10.0053
XX= 29.0044 YX= -2.2007 ZX= 2.8371
XY= -2.1958 YY= 18.6623 ZY= -1.2568

XZ= 2.4555 YZ= -1.2304 ZZ= 24.6636
Eigenvalues: 18.1325 23.4175 30.7803
23 H Isotropic = 24.1540 Anisotropy = 10.4963
XX= 27.9463 YX= -1.2680 ZX= -4.0851
XY= -1.3400 YY= 17.8829 ZY= -0.4522
XZ= -3.4541 YZ= -0.5295 ZZ= 26.6329
Eigenvalues: 17.5969 23.7137 31.1516
24 H Isotropic = 22.7971 Anisotropy = 10.3999
XX= 28.5978 YX= -2.0176 ZX= -2.4769
XY= -2.1046 YY= 15.9771 ZY= -0.7521
XZ= -2.1427 YZ= -0.7168 ZZ= 23.8165
Eigenvalues: 15.5003 23.1607 29.7304
25 H Isotropic = 23.9472 Anisotropy = 9.0560
XX= 27.0812 YX= -2.0796 ZX= 1.0273
XY= -2.1219 YY= 16.0254 ZY= -1.7673
XZ= 1.6512 YZ= -1.9012 ZZ= 28.7349
Eigenvalues: 15.4528 26.4043 29.9845
26 H Isotropic = 22.6877 Anisotropy = 16.3030
XX= 32.3122 YX= -3.2780 ZX= 4.0026
XY= -2.9683 YY= 13.5894 ZY= -1.6291
XZ= 1.3777 YZ= -1.3151 ZZ= 22.1614
Eigenvalues: 12.9632 21.5435 33.5564
27 H Isotropic = 22.8687 Anisotropy = 7.6809
XX= 26.5965 YX= -1.6681 ZX= -1.4024
XY= -1.7382 YY= 15.2392 ZY= -2.1163
XZ= -1.1785 YZ= -2.0382 ZZ= 26.7703
Eigenvalues: 14.5743 26.0424 27.9893
28 H Isotropic = 24.6024 Anisotropy = 3.6532
XX= 26.3151 YX= -0.8275 ZX= -0.0867
XY= -1.0609 YY= 21.3623 ZY= -0.9254
XZ= 1.0351 YZ= -1.0921 ZZ= 26.1298
Eigenvalues: 21.0251 25.7443 27.0379
29 H Isotropic = 25.0577 Anisotropy = 3.3524
XX= 26.6095 YX= -0.7917 ZX= 0.3175
XY= -0.8790 YY= 22.3091 ZY= -0.8231
XZ= 0.7862 YZ= -0.8913 ZZ= 26.2545
Eigenvalues: 22.0196 25.8608 27.2926
30 H Isotropic = 23.8180 Anisotropy = 13.5638
XX= 30.0061 YX= -2.7653 ZX= 4.1063
XY= -2.7608 YY= 17.5853 ZY= -1.8831
XZ= 4.2970 YZ= -1.8901 ZZ= 23.8624
Eigenvalues: 16.8284 21.7650 32.8605

Isomer 6 (conformer 2)

1 C Isotropic = 58.8705 Anisotropy = 143.3086
XX= 46.2553 YX= -19.3554 ZX= 28.0016
XY= -21.0965 YY= 129.3892 ZY= 61.3259
XZ= 31.5171 YZ= 60.8883 ZZ= 0.9669
Eigenvalues: -38.1477 60.3496 154.4095
2 C Isotropic = 47.6485 Anisotropy = 111.9776
XX= -39.3595 YX= -12.4471 ZX= -4.7187
XY= -13.4441 YY= 113.7240 ZY= 19.6644
XZ= -9.0391 YZ= 19.3743 ZZ= 68.5812
Eigenvalues: -40.7020 61.3474 122.3003
3 C Isotropic = 70.1046 Anisotropy = 124.7752
XX= 37.5394 YX= 2.3665 ZX= -34.0676
XY= 3.4250 YY= 140.0683 ZY= 37.3749
XZ= -40.3409 YZ= 40.0673 ZZ= 32.7062
Eigenvalues: -8.6257 65.6515 153.2881
4 C Isotropic = 46.7661 Anisotropy = 141.7542
XX= 20.4001 YX= -15.5671 ZX= 17.9037
XY= -17.3356 YY= 122.2464 ZY= 51.5157
XZ= 17.9316 YZ= 50.6407 ZZ= -2.3481
Eigenvalues: -30.5670 29.5965 141.2690
5 C Isotropic = 57.5271 Anisotropy = 169.0457
XX= -9.7569 YX= -10.9839 ZX= -7.7466
XY= -6.7187 YY= 150.7939 ZY= 49.8062
XZ= -9.5928 YZ= 51.8359 ZZ= 31.5444
Eigenvalues: -11.5208 13.8779 170.2242
6 C Isotropic = 59.1666 Anisotropy = 173.5453
XX= 29.7520 YX= 2.0884 ZX= -28.1053
XY= 6.5666 YY= 149.1617 ZY= 66.6199
XZ= -25.3977 YZ= 67.3657 ZZ= -1.4137
Eigenvalues: -37.4147 40.0511 174.8635
7 N Isotropic = 115.4283 Anisotropy = 86.8783
XX= 123.4597 YX= -0.5747 ZX= -9.5658
XY= -0.0078 YY= 157.6919 ZY= 42.9050
XZ= -20.4213 YZ= 37.5028 ZZ= 65.1335
Eigenvalues: 47.5403 125.3975 173.3472
8 C Isotropic = 59.6554 Anisotropy = 113.9075
XX= -12.3215 YX= -17.7514 ZX= 17.1348
XY= -8.4888 YY= 123.1678 ZY= 30.6958
XZ= 8.9208 YZ= 26.2771 ZZ= 68.1199
Eigenvalues: -16.6732 60.0456 135.5937
9 C Isotropic = 75.4366 Anisotropy = 109.3177
XX= 8.2491 YX= -0.5600 ZX= -16.5251
XY= 1.7049 YY= 138.3767 ZY= 27.2948
XZ= -9.4656 YZ= 24.5779 ZZ= 79.6840
Eigenvalues: 5.7517 72.2430 148.3151
10 C Isotropic = 21.1716 Anisotropy = 132.6559
XX= -2.6634 YX= 25.2449 ZX= -74.9411
XY= 41.3605 YY= 78.3420 ZY= -15.8519
XZ= -53.0092 YZ= -31.6310 ZZ= -12.1637
Eigenvalues: -71.7665 25.6724 109.6089
11 Br Isotropic = 1898.7868 Anisotropy = 1575.0805
XX= 2934.2854 YX= 153.9088 ZX= -16.4597
XY= 150.7629 YY= 1346.9405 ZY= -29.6368

XZ= 2.2025 YZ= -35.9557 ZZ= 1415.1347
Eigenvalues: 1321.5245 1425.9955 2948.8405
12 C Isotropic = 94.9092 Anisotropy = 41.0205
XX= 108.7368 YX= 17.0781 ZX= 15.7793
XY= 25.9646 YY= 87.9964 ZY= -30.0907
XZ= 26.5477 YZ= -37.2870 ZZ= 87.9943
Eigenvalues: 40.8808 121.5905 122.2562
13 C Isotropic = 19.6016 Anisotropy = 122.3422
XX= 28.6364 YX= 28.7970 ZX= -18.9956
XY= 20.1633 YY= 57.0517 ZY= -62.9328
XZ= -34.5712 YZ= -49.1511 ZZ= -26.8833
Eigenvalues: -57.1043 14.7460 101.1631
14 O Isotropic = -43.9763 Anisotropy = 258.7315
XX= -70.7602 YX= 86.7152 ZX= -41.9584
XY= 97.1897 YY= 19.7093 ZY= -103.9784
XZ= -47.7381 YZ= -84.6535 ZZ= -80.8780
Eigenvalues: -140.9726 -119.4676 128.5114
15 N Isotropic = -129.3858 Anisotropy = 259.8454
XX= -206.5532 YX= 74.1811 ZX= -121.5852
XY= 95.9291 YY= -21.9683 ZY= -21.7870
XZ= -117.3816 YZ= -44.1148 ZZ= -159.6359
Eigenvalues: -312.4067 -119.5952 43.8444
16 C Isotropic = 62.7535 Anisotropy = 101.2968
XX= 28.4389 YX= 36.4272 ZX= -31.0812
XY= 40.6937 YY= 99.4065 ZY= -19.5291
XZ= -24.8805 YZ= -22.9142 ZZ= 60.4151
Eigenvalues: 5.2592 52.7166 130.2847
17 N Isotropic = 97.9084 Anisotropy = 126.3683
XX= 94.4047 YX= 54.1271 ZX= 18.0045
XY= 51.6254 YY= 123.5416 ZY= -63.8028
XZ= 14.7542 YZ= -61.0798 ZZ= 75.7789
Eigenvalues: 8.6726 102.8986 182.1539
18 C Isotropic = 62.6639 Anisotropy = 120.4501
XX= 25.0559 YX= 38.4742 ZX= -44.4226
XY= 35.7713 YY= 112.9279 ZY= -22.9836
XZ= -50.3008 YZ= -20.8549 ZZ= 50.0080
Eigenvalues: -13.7643 58.7921 142.9640
19 C Isotropic = 71.4730 Anisotropy = 135.5607
XX= 71.5094 YX= 28.0145 ZX= -37.0880
XY= 29.4164 YY= 121.0031 ZY= -51.0750
XZ= -34.2670 YZ= -52.5992 ZZ= 21.9065
Eigenvalues: -7.0908 59.6630 161.8468
20 C Isotropic = 69.1777 Anisotropy = 144.9301
XX= 39.1673 YX= 60.7397 ZX= -8.7463
XY= 60.6294 YY= 108.1347 ZY= -52.1789
XZ= -5.4075 YZ= -50.6913 ZZ= 60.2311
Eigenvalues: -4.1492 45.8846 165.7978
21 I Isotropic = 3878.7920 Anisotropy = 1564.7990
XX= 3760.6913 YX= -470.0250 ZX= -630.2524
XY= -483.7515 YY= 4278.0730 ZY= 415.4025
XZ= -625.2054 YZ= 397.7913 ZZ= 3597.6115
Eigenvalues: 3046.0554 3668.3292 4921.9913
22 H Isotropic = 24.2206 Anisotropy = 10.4475
XX= 29.3700 YX= 0.2704 ZX= 3.8122
XY= 0.9970 YY= 19.0824 ZY= -1.9217

XZ= 3.2911 YZ= -1.7195 ZZ= 24.2094
Eigenvalues: 18.2071 23.2691 31.1856
23 H Isotropic = 24.0946 Anisotropy = 9.7424
XX= 28.3267 YX= 2.0656 ZX= -2.8090
XY= 1.9924 YY= 18.6836 ZY= -2.6708
XZ= -2.2993 YZ= -2.6565 ZZ= 25.2735
Eigenvalues: 17.6242 24.0701 30.5895
24 H Isotropic = 23.8142 Anisotropy = 11.3016
XX= 28.8163 YX= 4.2618 ZX= -0.0662
XY= 5.9935 YY= 20.8633 ZY= -0.4110
XZ= -0.6469 YZ= -0.1201 ZZ= 21.7630
Eigenvalues: 18.3490 21.7450 31.3486
25 H Isotropic = 23.8889 Anisotropy = 9.9926
XX= 25.7106 YX= 0.2323 ZX= 1.3166
XY= -0.0784 YY= 17.0148 ZY= -3.6353
XZ= 2.0435 YZ= -3.8718 ZZ= 28.9413
Eigenvalues: 15.9015 25.2145 30.5506
26 H Isotropic = 24.2038 Anisotropy = 5.5796
XX= 25.2201 YX= -0.2320 ZX= 0.5549
XY= -0.2791 YY= 20.2284 ZY= -3.1194
XZ= 0.0896 YZ= -1.5272 ZZ= 27.1628
Eigenvalues: 19.5180 25.1698 27.9235
27 H Isotropic = 22.9303 Anisotropy = 7.4278
XX= 24.4713 YX= -4.1457 ZX= 1.3708
XY= -4.0890 YY= 19.1766 ZY= 4.3377
XZ= 1.0052 YZ= 4.4248 ZZ= 25.1430
Eigenvalues: 14.9909 25.9178 27.8821
28 H Isotropic = 24.6010 Anisotropy = 3.6729
XX= 25.9163 YX= -1.5370 ZX= 1.8177
XY= -1.9499 YY= 22.6627 ZY= 1.1000
XZ= 0.8203 YZ= 1.5509 ZZ= 25.2238
Eigenvalues: 21.1458 25.6075 27.0496
29 H Isotropic = 25.0719 Anisotropy = 3.3788
XX= 26.2040 YX= -1.3667 ZX= 1.4811
XY= -1.4788 YY= 23.3598 ZY= 1.0221
XZ= 1.1255 YZ= 1.1250 ZZ= 25.6519
Eigenvalues: 22.1168 25.7744 27.3244
30 H Isotropic = 23.8532 Anisotropy = 13.3192
XX= 26.7408 YX= -2.2574 ZX= 6.3355
XY= -1.9213 YY= 18.7300 ZY= 1.2040
XZ= 6.1905 YZ= 0.8893 ZZ= 26.0888
Eigenvalues: 17.1018 21.7252 32.7326

Isomer 6 (conformer 3)

1 C Isotropic = 56.9931 Anisotropy = 144.7005
XX= 52.0896 YX= 15.2340 ZX= 31.0228
XY= 14.9245 YY= 147.8879 ZY= 19.0722
XZ= 33.4140 YZ= 19.2317 ZZ= -28.9981
Eigenvalues: -41.1702 58.6895 153.4601
2 C Isotropic = 46.6606 Anisotropy = 113.1693
XX= -36.0356 YX= 28.7692 ZX= 11.8009
XY= 29.9447 YY= 115.4822 ZY= 6.0713
XZ= 8.1083 YZ= 7.1569 ZZ= 60.5352
Eigenvalues: -42.2422 60.1172 122.1068
3 C Isotropic = 71.0583 Anisotropy = 123.3893
XX= 37.0818 YX= 27.1098 ZX= -32.0859
XY= 27.6728 YY= 144.6479 ZY= 23.3061
XZ= -36.3256 YZ= 24.2899 ZZ= 31.4452
Eigenvalues: -8.5578 68.4149 153.3179
4 C Isotropic = 47.1137 Anisotropy = 141.9452
XX= 28.1103 YX= 19.1228 ZX= 21.2836
XY= 18.4178 YY= 135.5188 ZY= 18.7222
XZ= 22.3405 YZ= 18.7676 ZZ= -22.2881
Eigenvalues: -31.1839 30.7811 141.7438
5 C Isotropic = 57.9650 Anisotropy = 162.8847
XX= -5.8026 YX= 33.5730 ZX= 0.5807
XY= 33.8219 YY= 156.8399 ZY= 22.1095
XZ= -1.1316 YZ= 20.3917 ZZ= 22.8577
Eigenvalues: -13.0903 20.4305 166.5548
6 C Isotropic = 56.0378 Anisotropy = 175.5714
XX= 25.2041 YX= 32.2976 ZX= -25.5487
XY= 30.0539 YY= 162.5592 ZY= 33.2282
XZ= -21.6778 YZ= 31.3954 ZZ= -19.6499
Eigenvalues: -38.7012 33.7292 173.0854
7 N Isotropic = 115.4854 Anisotropy = 83.1974
XX= 124.7076 YX= 11.5898 ZX= -17.3692
XY= 12.7269 YY= 165.9326 ZY= 18.0622
XZ= -24.1080 YZ= 20.6080 ZZ= 55.8159
Eigenvalues: 46.0432 129.4626 170.9503
8 C Isotropic = 60.0117 Anisotropy = 121.5947
XX= 0.6206 YX= 24.0210 ZX= 27.7137
XY= 27.3641 YY= 134.4817 ZY= 8.1508
XZ= 14.1131 YZ= 10.7412 ZZ= 44.9327
Eigenvalues: -10.6613 49.6215 141.0748
9 C Isotropic = 74.6959 Anisotropy = 110.8595
XX= 19.6042 YX= 26.7959 ZX= -4.9124
XY= 24.5522 YY= 141.6104 ZY= 13.8480
XZ= 3.2513 YZ= 11.8862 ZZ= 62.8731
Eigenvalues: 14.1841 61.3013 148.6023
10 C Isotropic = 24.5948 Anisotropy = 132.1921
XX= -48.6534 YX= 30.5776 ZX= -6.3784
XY= 37.3254 YY= 102.3642 ZY= 18.4861
XZ= -36.9438 YZ= 24.6039 ZZ= 20.0737
Eigenvalues: -63.9449 25.0065 112.7229
11 Br Isotropic = 1902.9764 Anisotropy = 1572.1415
XX= 2873.5452 YX= -264.8975 ZX= -220.1561
XY= -275.6255 YY= 1378.7575 ZY= 24.1903

XZ= -202.9025 YZ= 21.5514 ZZ= 1456.6263
Eigenvalues: 1329.4161 1428.4423 2951.0707
12 C Isotropic = 105.8437 Anisotropy = 48.3257
XX= 111.7378 YX= -6.1490 ZX= 42.1997
XY= -5.1820 YY= 125.8986 ZY= 0.1547
XZ= 33.4105 YZ= 3.1030 ZZ= 79.8945
Eigenvalues: 54.5119 124.9582 138.0608
13 C Isotropic = 20.4867 Anisotropy = 122.9206
XX= -46.8706 YX= 24.4984 ZX= 16.6308
XY= 20.4622 YY= 95.8932 ZY= 14.1252
XZ= 32.7650 YZ= 11.3683 ZZ= 12.4375
Eigenvalues: -57.7066 16.7330 102.4338
14 O Isotropic = -41.6837 Anisotropy = 254.8558
XX= -119.6805 YX= 45.8669 ZX= 0.3161
XY= 42.2811 YY= 110.9774 ZY= 48.7516
XZ= 10.4420 YZ= 45.2428 ZZ= -116.3479
Eigenvalues: -130.0295 -123.2417 128.2202
15 N Isotropic = -126.6053 Anisotropy = 263.5257
XX= -235.1444 YX= 66.4995 ZX= -71.1456
XY= 68.8171 YY= 25.4400 ZY= 56.3279
XZ= -91.8608 YZ= 59.2875 ZZ= -170.1115
Eigenvalues: -313.4886 -115.4058 49.0785
16 C Isotropic = 62.1738 Anisotropy = 99.2220
XX= 11.5134 YX= 18.3158 ZX= 20.2318
XY= 17.7180 YY= 123.0219 ZY= 10.3721
XZ= 25.8896 YZ= 9.4182 ZZ= 51.9861
Eigenvalues: -0.2094 58.4090 128.3218
17 N Isotropic = 94.8844 Anisotropy = 135.5917
XX= 90.6954 YX= 14.6432 ZX= 16.9165
XY= 14.7315 YY= 177.1218 ZY= 28.4645
XZ= 13.7595 YZ= 29.2287 ZZ= 16.8360
Eigenvalues: 9.8026 89.5717 185.2788
18 C Isotropic = 63.1712 Anisotropy = 117.6186
XX= -8.6863 YX= 25.4297 ZX= 16.8291
XY= 27.3920 YY= 134.1981 ZY= 11.5338
XZ= 6.1243 YZ= 13.4458 ZZ= 64.0018
Eigenvalues: -14.4846 62.4146 141.5836
19 C Isotropic = 71.5951 Anisotropy = 138.3401
XX= 25.6835 YX= 31.1070 ZX= -25.7934
XY= 31.0971 YY= 152.4904 ZY= 28.7774
XZ= -24.8399 YZ= 28.6916 ZZ= 36.6114
Eigenvalues: -6.0222 56.9857 163.8219
20 C Isotropic = 68.8486 Anisotropy = 142.4366
XX= 40.0030 YX= 18.3874 ZX= 27.8775
XY= 18.6110 YY= 155.8036 ZY= 23.6263
XZ= 27.2090 YZ= 23.6312 ZZ= 10.7394
Eigenvalues: -6.5838 49.3234 163.8064
21 I Isotropic = 3930.2297 Anisotropy = 1444.2212
XX= 3407.8600 YX= 211.2940 ZX= -671.1509
XY= 202.4096 YY= 3780.6085 ZY= -55.6520
XZ= -595.4085 YZ= -68.1640 ZZ= 4602.2207
Eigenvalues: 3094.1124 3803.5329 4893.0439
22 H Isotropic = 24.0882 Anisotropy = 10.0092
XX= 28.9546 YX= -2.4843 ZX= 2.7101
XY= -2.4563 YY= 18.8017 ZY= -1.4280

XZ= 2.3299 YZ= -1.3729 ZZ= 24.5084
Eigenvalues: 18.1209 23.3828 30.7610
 23 H Isotropic = 24.1576 Anisotropy = 10.4783
XX= 27.8123 YX= -1.3865 ZX= -4.1166
XY= -1.4773 YY= 17.9559 ZY= -0.5307
XZ= -3.4957 YZ= -0.6236 ZZ= 26.7048
Eigenvalues: 17.5949 23.7349 31.1432
 24 H Isotropic = 22.7800 Anisotropy = 10.3604
XX= 28.3912 YX= -2.1960 ZX= -2.5976
XY= -2.2980 YY= 16.1094 ZY= -0.8416
XZ= -2.3034 YZ= -0.8030 ZZ= 23.8394
Eigenvalues: 15.5183 23.1348 29.6869
 25 H Isotropic = 23.9703 Anisotropy = 9.0727
XX= 27.0556 YX= -2.3370 ZX= 0.9740
XY= -2.3933 YY= 16.2192 ZY= -2.0275
XZ= 1.6046 YZ= -2.1717 ZZ= 28.6361
Eigenvalues: 15.4771 26.4151 30.0188
 26 H Isotropic = 22.8910 Anisotropy = 16.1130
XX= 32.2865 YX= -3.6871 ZX= 3.8406
XY= -3.3512 YY= 14.1650 ZY= -1.8107
XZ= 1.2299 YZ= -1.4523 ZZ= 22.2216
Eigenvalues: 13.3531 21.6870 33.6330
 27 H Isotropic = 21.5943 Anisotropy = 20.0183
XX= 27.7170 YX= -4.7446 ZX= 5.6517
XY= -4.8513 YY= 10.6762 ZY= -4.4149
XZ= 6.4863 YZ= -4.5778 ZZ= 26.3897
Eigenvalues: 8.8934 20.9497 34.9398
 28 H Isotropic = 24.6090 Anisotropy = 4.2917
XX= 26.8818 YX= -1.3856 ZX= 1.1536
XY= -1.1470 YY= 21.2197 ZY= -1.1482
XZ= -0.1229 YZ= -0.9033 ZZ= 25.7253
Eigenvalues: 20.7843 25.5724 27.4701
 29 H Isotropic = 25.0941 Anisotropy = 2.7232
XX= 26.4949 YX= -0.9129 ZX= 0.4712
XY= -0.8183 YY= 22.5077 ZY= -0.8599
XZ= -0.0989 YZ= -0.7442 ZZ= 26.2798
Eigenvalues: 22.1904 26.1824 26.9096
 30 H Isotropic = 24.2417 Anisotropy = 5.4664
XX= 26.5120 YX= -1.4230 ZX= 0.9533
XY= -1.5321 YY= 20.4615 ZY= -1.2567
XZ= 1.3966 YZ= -1.3510 ZZ= 25.7516
Eigenvalues: 19.9365 24.9025 27.8860

Isomer 6 (conformer 4)

1 C Isotropic = 58.8437 Anisotropy = 143.5225
XX= 57.4106 YX= -22.6355 ZX= 15.2603
XY= -23.7803 YY= 133.6668 ZY= 54.5772
XZ= 19.0175 YZ= 54.4625 ZZ= -14.5464
Eigenvalues: -38.3110 60.3167 154.5253
2 C Isotropic = 47.4141 Anisotropy = 112.3502
XX= -33.6053 YX= -31.2584 ZX= 5.9896
XY= -32.9629 YY= 110.7048 ZY= 18.1153
XZ= 1.8589 YZ= 17.2744 ZZ= 65.1428
Eigenvalues: -40.9689 60.8970 122.3143
3 C Isotropic = 69.8906 Anisotropy = 125.1282
XX= 29.7639 YX= -12.8173 ZX= -37.8260
XY= -12.3007 YY= 144.3466 ZY= 23.3708
XZ= -44.4470 YZ= 24.8254 ZZ= 35.5613
Eigenvalues: -8.9377 65.3000 153.3093
4 C Isotropic = 46.8085 Anisotropy = 141.9566
XX= 28.7925 YX= -23.4164 ZX= 9.0417
XY= -25.1075 YY= 125.1421 ZY= 43.7531
XZ= 9.3235 YZ= 42.8687 ZZ= -13.5091
Eigenvalues: -30.1927 29.1720 141.4462
5 C Isotropic = 57.4175 Anisotropy = 169.1949
XX= -6.4930 YX= -29.6589 ZX= -8.5220
XY= -25.8967 YY= 153.7396 ZY= 39.4760
XZ= -10.6642 YZ= 41.2188 ZZ= 25.0060
Eigenvalues: -11.4602 13.4986 170.2141
6 C Isotropic = 59.7330 Anisotropy = 172.8000
XX= 24.1084 YX= -13.0484 ZX= -39.4973
XY= -8.6486 YY= 159.0460 ZY= 47.1584
XZ= -36.6464 YZ= 48.5030 ZZ= -3.9553
Eigenvalues: -36.5431 40.8091 174.9330
7 N Isotropic = 115.3496 Anisotropy = 87.6016
XX= 119.1917 YX= -4.2281 ZX= -21.3039
XY= -3.7948 YY= 163.5555 ZY= 33.0669
XZ= -31.0962 YZ= 25.3349 ZZ= 63.3014
Eigenvalues: 47.1489 125.1491 173.7507
8 C Isotropic = 59.6650 Anisotropy = 114.0521
XX= -3.4987 YX= -32.2702 ZX= 22.7897
XY= -23.1006 YY= 122.5509 ZY= 29.3698
XZ= 13.6568 YZ= 25.2388 ZZ= 59.9428
Eigenvalues: -16.8272 60.1226 135.6997
9 C Isotropic = 75.5321 Anisotropy = 109.2439
XX= 8.3423 YX= -18.6960 ZX= -11.0798
XY= -15.7455 YY= 140.2498 ZY= 20.0222
XZ= -4.1753 YZ= 19.0504 ZZ= 78.0043
Eigenvalues: 5.7587 72.4763 148.3614
10 C Isotropic = 22.2831 Anisotropy = 130.6776
XX= -19.8351 YX= -0.8928 ZX= -72.0585
XY= 19.1074 YY= 78.9272 ZY= -36.9283
XZ= -48.7516 YZ= -48.1539 ZZ= 7.7571
Eigenvalues: -70.7331 28.1808 109.4015
11 Br Isotropic = 1898.4110 Anisotropy = 1582.6376
XX= 2848.0408 YX= 351.4588 ZX= -192.9778
XY= 346.7747 YY= 1404.7844 ZY= -71.5831

XZ= -176.1062 YZ= -73.3262 ZZ= 1442.4079
Eigenvalues: 1316.3179 1425.4125 2953.5028
12 C Isotropic = 99.2860 Anisotropy = 49.8514
XX= 112.8091 YX= 18.0363 ZX= 20.2829
XY= 27.7920 YY= 88.4025 ZY= -29.6963
XZ= 32.9001 YZ= -32.3047 ZZ= 96.6464
Eigenvalues: 43.6950 121.6427 132.5203
13 C Isotropic = 18.9452 Anisotropy = 124.0922
XX= 16.5451 YX= 15.1032 ZX= -18.4608
XY= 6.1339 YY= 50.2092 ZY= -73.9472
XZ= -31.3202 YZ= -64.4847 ZZ= -9.9187
Eigenvalues: -58.4513 13.6136 101.6734
14 O Isotropic = -54.5609 Anisotropy = 265.0704
XX= -113.3164 YX= 54.3839 ZX= -37.5443
XY= 64.6255 YY= 14.5445 ZY= -126.3617
XZ= -41.2460 YZ= -112.2348 ZZ= -64.9108
Eigenvalues: -151.3750 -134.4604 122.1527
15 N Isotropic = -132.5450 Anisotropy = 268.6333
XX= -257.4788 YX= 25.4721 ZX= -116.7136
XY= 48.6472 YY= -11.3318 ZY= -59.3243
XZ= -107.0376 YZ= -82.6422 ZZ= -128.8245
Eigenvalues: -322.2446 -121.9343 46.5438
16 C Isotropic = 62.2964 Anisotropy = 100.1156
XX= 63.0545 YX= 12.9409 ZX= -15.1704
XY= 10.7164 YY= 84.3628 ZY= -57.8649
XZ= -19.9665 YZ= -56.0476 ZZ= 39.4720
Eigenvalues: -0.3289 58.1781 129.0401
17 N Isotropic = 94.5784 Anisotropy = 136.0897
XX= 50.4453 YX= 52.0224 ZX= 5.4587
XY= 54.0773 YY= 124.7895 ZY= -58.3372
XZ= 9.8258 YZ= -57.7280 ZZ= 108.5005
Eigenvalues: 9.2885 89.1419 185.3049
18 C Isotropic = 63.0273 Anisotropy = 118.2907
XX= 56.6241 YX= 1.3445 ZX= -41.2945
XY= 7.9646 YY= 96.3469 ZY= -60.6339
XZ= -32.5647 YZ= -62.8635 ZZ= 36.1108
Eigenvalues: -14.7693 61.9633 141.8878
19 C Isotropic = 71.7478 Anisotropy = 137.9432
XX= 14.2372 YX= 24.4634 ZX= -40.7496
XY= 24.3006 YY= 123.1352 ZY= -45.4453
XZ= -41.4316 YZ= -45.6116 ZZ= 77.8711
Eigenvalues: -5.9475 57.4810 163.7099
20 C Isotropic = 69.4205 Anisotropy = 142.5901
XX= 44.5018 YX= 42.3426 ZX= -0.6167
XY= 42.3732 YY= 99.9823 ZY= -70.1437
XZ= 0.3121 YZ= -71.0178 ZZ= 63.7776
Eigenvalues: -6.2510 50.0320 164.4806
21 I Isotropic = 3921.4883 Anisotropy = 1531.2993
XX= 3798.6746 YX= -568.2029 ZX= -648.0380
XY= -522.3454 YY= 4244.6222 ZY= 275.5069
XZ= -673.8844 YZ= 306.4580 ZZ= 3721.1681
Eigenvalues: 3068.9267 3753.1837 4942.3546
22 H Isotropic = 24.1960 Anisotropy = 10.4339
XX= 29.6498 YX= 1.9337 ZX= 3.3317
XY= 2.5511 YY= 19.2392 ZY= -1.1630

XZ= 2.7073 YZ= -0.9682 ZZ= 23.6989
Eigenvalues: 18.2134 23.2226 31.1519
23 H Isotropic = 24.0836 Anisotropy = 9.7479
XX= 27.0360 YX= 2.7834 ZX= -2.8797
XY= 2.7541 YY= 18.9065 ZY= -2.7085
XZ= -2.3696 YZ= -2.6120 ZZ= 26.3082
Eigenvalues: 17.6418 24.0268 30.5821
24 H Isotropic = 23.8291 Anisotropy = 11.1547
XX= 27.0326 YX= 5.0623 ZX= -1.0558
XY= 6.5381 YY= 22.3457 ZY= -1.1569
XZ= -1.7471 YZ= -0.8163 ZZ= 22.1090
Eigenvalues: 18.4331 21.7886 31.2655
25 H Isotropic = 23.8154 Anisotropy = 9.9760
XX= 25.8968 YX= 1.3793 ZX= 1.9848
XY= 1.1956 YY= 16.5465 ZY= -2.2456
XZ= 2.7853 YZ= -2.5393 ZZ= 29.0028
Eigenvalues: 15.8066 25.1735 30.4661
26 H Isotropic = 24.1990 Anisotropy = 5.6296
XX= 25.2240 YX= 0.4771 ZX= 1.1560
XY= 0.4048 YY= 19.9186 ZY= -2.3760
XZ= 0.3628 YZ= -0.8891 ZZ= 27.4544
Eigenvalues: 19.5194 25.1255 27.9521
27 H Isotropic = 21.6429 Anisotropy = 19.6539
XX= 31.5679 YX= -2.9947 ZX= 7.1158
XY= -2.9827 YY= 13.6799 ZY= 4.9062
XZ= 6.6512 YZ= 4.6935 ZZ= 19.6811
Eigenvalues: 9.3058 20.8775 34.7455
28 H Isotropic = 24.5885 Anisotropy = 4.3424
XX= 26.4078 YX= -1.1503 ZX= 1.0724
XY= -0.2649 YY= 22.5611 ZY= 2.3704
XZ= 2.1538 YZ= 1.9367 ZZ= 24.7966
Eigenvalues: 20.8636 25.4185 27.4835
29 H Isotropic = 25.1032 Anisotropy = 2.6960
XX= 26.4873 YX= -0.9943 ZX= 0.6173
XY= -0.5747 YY= 23.6860 ZY= 1.7448
XZ= 1.0905 YZ= 1.5082 ZZ= 25.1364
Eigenvalues: 22.3258 26.0833 26.9006
30 H Isotropic = 24.2803 Anisotropy = 5.2743
XX= 26.9250 YX= -0.8298 ZX= 2.0269
XY= -1.1533 YY= 21.8214 ZY= 1.8392
XZ= 1.5625 YZ= 1.8963 ZZ= 24.0945
Eigenvalues: 20.2957 24.7487 27.7965

Isomer 7 (conformer 1)

1 C Isotropic = 56.2147 Anisotropy = 146.6191
XX= 42.0012 YX= 46.0439 ZX= 44.9147
XY= 46.6089 YY= 134.7886 ZY= -19.5845
XZ= 42.2643 YZ= -17.8962 ZZ= -8.1456
Eigenvalues: -42.5654 57.2488 153.9608
2 C Isotropic = 46.2622 Anisotropy = 115.5214
XX= 42.3980 YX= 32.8718 ZX= -44.0648
XY= 32.7427 YY= 109.9636 ZY= 16.9194
XZ= -40.5487 YZ= 15.8861 ZZ= -13.5751
Eigenvalues: -42.3796 57.8897 123.2764
3 C Isotropic = 70.3969 Anisotropy = 124.8127
XX= 14.7915 YX= 56.5887 ZX= -11.6021
XY= 56.5274 YY= 130.5579 ZY= 3.9633
XZ= -7.2652 YZ= 2.5976 ZZ= 65.8415
Eigenvalues: -9.5722 67.1575 153.6054
4 C Isotropic = 47.0099 Anisotropy = 138.9095
XX= 29.9578 YX= 45.3448 ZX= 28.1624
XY= 46.4997 YY= 120.3849 ZY= -11.4824
XZ= 26.3157 YZ= -11.6532 ZZ= -9.3130
Eigenvalues: -30.5368 31.9503 139.6162
5 C Isotropic = 59.6673 Anisotropy = 162.6985
XX= 30.5273 YX= 56.6480 ZX= -16.4686
XY= 55.7256 YY= 145.1906 ZY= 6.4610
XZ= -15.4234 YZ= 6.1144 ZZ= 3.2839
Eigenvalues: -11.8396 22.7085 168.1330
6 C Isotropic = 58.4864 Anisotropy = 172.5195
XX= -4.9535 YX= 72.9579 ZX= 13.8016
XY= 73.4648 YY= 143.4618 ZY= -4.3549
XZ= 8.9765 YZ= -3.9028 ZZ= 36.9508
Eigenvalues: -36.9712 38.9309 173.4994
7 N Isotropic = 111.5959 Anisotropy = 89.4817
XX= 65.8722 YX= 43.6341 ZX= 21.6431
XY= 40.5180 YY= 154.4412 ZY= -9.2026
XZ= 28.6349 YZ= -12.2059 ZZ= 114.4743
Eigenvalues: 39.1625 124.3749 171.2504
8 C Isotropic = 59.9962 Anisotropy = 119.6866
XX= 54.2764 YX= 34.8226 ZX= -21.4530
XY= 26.4483 YY= 128.7994 ZY= 5.2405
XZ= -10.3658 YZ= 3.5402 ZZ= -3.0874
Eigenvalues: -8.3427 48.5439 139.7872
9 C Isotropic = 76.1568 Anisotropy = 108.8366
XX= 60.3159 YX= 35.7012 ZX= -15.7638
XY= 34.7455 YY= 134.6792 ZY= 6.7849
XZ= -24.5261 YZ= 9.5723 ZZ= 33.4753
Eigenvalues: 17.2133 62.5426 148.7145
10 C Isotropic = 16.5680 Anisotropy = 123.6574
XX= -34.2580 YX= 46.9325 ZX= -3.5644
XY= 47.6541 YY= 82.0437 ZY= 3.3887
XZ= 19.7662 YZ= -0.8243 ZZ= 1.9183
Eigenvalues: -52.0256 2.7233 99.0063
11 Br Isotropic = 1885.9428 Anisotropy = 1576.8179
XX= 1704.8448 YX= -155.8422 ZX= 613.1009
XY= -153.4682 YY= 1374.4529 ZY= -238.5470
XZ= 593.7409 YZ= -234.3579 ZZ= 2578.5306
Eigenvalues: 1313.3476 1407.3260 2937.1547
12 C Isotropic = 73.5635 Anisotropy = 77.7692
XX= 50.8479 YX= 21.9272 ZX= 28.3615

XY= 21.0831 YY= 119.2040 ZY= -10.5588
XZ= 20.2287 YZ= -2.5356 ZZ= 50.6387
Eigenvalues: 22.3053 72.9757 125.4097
 13 C Isotropic = 26.9646 Anisotropy = 79.0596
XX= -6.5180 YX= 31.6506 ZX= -41.9472
XY= 41.0427 YY= 64.3430 ZY= 17.5818
XZ= -69.8283 YZ= 29.4219 ZZ= 23.0687
Eigenvalues: -64.0422 65.2650 79.6710
 14 N Isotropic = -134.4400 Anisotropy = 263.8457
XX= -194.5563 YX= 85.1551 ZX= -75.0197
XY= 90.2532 YY= 7.6550 ZY= 52.0372
XZ= -93.9986 YZ= 43.9729 ZZ= -216.4185
Eigenvalues: -318.2851 -126.4919 41.4572
 15 O Isotropic = -75.3456 Anisotropy = 276.9556
XX= -140.4574 YX= 85.0715 ZX= 50.1213
XY= 87.5990 YY= 78.2980 ZY= 2.7412
XZ= 54.2071 YZ= -4.0958 ZZ= -163.8773
Eigenvalues: -217.1523 -118.1759 109.2915
 16 I Isotropic = 3753.1729 Anisotropy = 2048.2321
XX= 3880.0171 YX= -238.8657 ZX= 1114.8070
XY= -283.2713 YY= 3478.5863 ZY= -441.4637
XZ= 1042.6125 YZ= -432.1998 ZZ= 3900.9152
Eigenvalues: 2786.1176 3354.7400 5118.6609
 17 C Isotropic = 63.9244 Anisotropy = 107.9054
XX= 49.7165 YX= -44.2608 ZX= 54.1653
XY= -42.1886 YY= 87.9679 ZY= -10.2270
XZ= 49.1615 YZ= -10.8897 ZZ= 54.0889
Eigenvalues: -6.7733 62.6852 135.8614
 18 N Isotropic = 93.2843 Anisotropy = 115.8752
XX= 112.3714 YX= -55.4383 ZX= -8.1685
XY= -51.3529 YY= 83.7734 ZY= -64.6518
XZ= 1.4437 YZ= -55.8838 ZZ= 83.7081
Eigenvalues: 6.7828 102.5358 170.5344
 19 C Isotropic = 66.5357 Anisotropy = 116.6272
XX= 55.2867 YX= -41.6920 ZX= 53.8394
XY= -39.8569 YY= 94.7589 ZY= -18.1264
XZ= 63.8327 YZ= -10.9639 ZZ= 49.5615
Eigenvalues: -9.8558 65.1757 144.2872
 20 C Isotropic = 70.8624 Anisotropy = 139.4517
XX= 91.2136 YX= -31.7847 ZX= 47.8022
XY= -36.8653 YY= 90.6970 ZY= -55.1748
XZ= 44.1244 YZ= -55.2802 ZZ= 30.6764
Eigenvalues: -8.3309 57.0878 163.8301
 21 C Isotropic = 69.6893 Anisotropy = 139.0434
XX= 59.3354 YX= -72.1478 ZX= 31.0222
XY= -74.1842 YY= 72.7628 ZY= -31.0956
XZ= 29.2135 YZ= -33.5848 ZZ= 76.9697
Eigenvalues: -7.4272 54.1101 162.3849
 22 H Isotropic = 24.0198 Anisotropy = 9.9883
XX= 27.3814 YX= -3.7312 ZX= 2.8302
XY= -3.6781 YY= 19.6203 ZY= -1.1922
XZ= 3.0765 YZ= -1.2311 ZZ= 25.0576
Eigenvalues: 18.1358 23.2449 30.6787
 23 H Isotropic = 24.1884 Anisotropy = 10.3658
XX= 22.9160 YX= -2.1192 ZX= 0.0137
XY= -2.1756 YY= 18.5700 ZY= -0.0624
XZ= -0.7185 YZ= 0.3458 ZZ= 31.0792
Eigenvalues: 17.6879 23.7783 31.0990

24 H Isotropic = 23.0109 Anisotropy = 10.2740
XX= 22.6487 YX= -2.4281 ZX= 2.0934
XY= -2.2439 YY= 17.0632 ZY= -0.7623
XZ= 1.3941 YZ= -0.4898 ZZ= 29.3208
Eigenvalues: 16.2150 22.9575 29.8603
25 H Isotropic = 24.0880 Anisotropy = 8.9261
XX= 27.7740 YX= -5.0350 ZX= 0.3622
XY= -5.4555 YY= 17.8900 ZY= -0.3764
XZ= -0.4732 YZ= 0.1878 ZZ= 26.5999
Eigenvalues: 15.6242 26.6010 30.0387
26 H Isotropic = 24.9213 Anisotropy = 12.6249
XX= 27.0066 YX= -4.2773 ZX= 3.7059
XY= -4.6814 YY= 19.8419 ZY= -4.6483
XZ= 3.5229 YZ= -2.0170 ZZ= 27.9153
Eigenvalues: 17.4478 23.9782 33.3379
27 H Isotropic = 24.1014 Anisotropy = 4.4073
XX= 23.7380 YX= 2.9714 ZX= -1.6803
XY= 3.7757 YY= 23.5904 ZY= 0.3847
XZ= -0.9603 YZ= 2.1954 ZZ= 24.9760
Eigenvalues: 19.6503 25.6144 27.0397
28 H Isotropic = 24.6955 Anisotropy = 3.9325
XX= 25.2421 YX= 1.2199 ZX= -2.3587
XY= 1.7523 YY= 23.1963 ZY= -0.3632
XZ= -1.1255 YZ= 1.2696 ZZ= 25.6480
Eigenvalues: 21.9630 24.8062 27.3171
29 H Isotropic = 25.0137 Anisotropy = 2.8316
XX= 25.2716 YX= 0.7437 ZX= -1.1561
XY= 0.7847 YY= 23.7595 ZY= 1.0020
XZ= -1.0020 YZ= 1.4135 ZZ= 26.0101
Eigenvalues: 22.7095 25.4303 26.9014
30 H Isotropic = 25.1129 Anisotropy = 5.9069
XX= 25.0007 YX= -1.3081 ZX= -0.8739
XY= -1.2009 YY= 24.6606 ZY= 4.1253
XZ= -1.4177 YZ= 2.1512 ZZ= 25.6775
Eigenvalues: 21.9723 24.3156 29.0509

Isomer 7 (conformer 2)

1 C Isotropic = 56.8466 Anisotropy = 145.3184
XX= 48.5525 YX= 44.9071 ZX= 28.2913
XY= 45.1529 YY= 120.8258 ZY= -55.7458
XZ= 27.5739 YZ= -57.0973 ZZ= 1.1614
Eigenvalues: -42.4226 59.2368 153.7255
2 C Isotropic = 46.3927 Anisotropy = 115.2356
XX= 25.3187 YX= 13.8658 ZX= -57.2120
XY= 15.3473 YY= 111.7207 ZY= -20.6003
XZ= -52.1518 YZ= -21.1669 ZZ= 2.1386
Eigenvalues: -42.5001 58.4617 123.2164
3 C Isotropic = 70.5878 Anisotropy = 124.2147
XX= 4.4458 YX= 42.6659 ZX= -15.1557
XY= 41.4831 YY= 134.1632 ZY= -19.5630
XZ= -10.0751 YZ= -21.5555 ZZ= 73.1544
Eigenvalues: -8.5077 66.8735 153.3976
4 C Isotropic = 46.7449 Anisotropy = 138.8505
XX= 28.1568 YX= 38.2574 ZX= 12.4952
XY= 37.6407 YY= 112.6588 ZY= -49.7850
XZ= 13.5331 YZ= -46.1705 ZZ= -0.5808
Eigenvalues: -30.3575 31.2804 139.3120
5 C Isotropic = 60.4541 Anisotropy = 161.7637
XX= 20.0271 YX= 39.3225 ZX= -30.8116
XY= 41.1948 YY= 143.2810 ZY= -36.1142
XZ= -30.1379 YZ= -37.4001 ZZ= 18.0542
Eigenvalues: -11.4740 24.5397 168.2966
6 C Isotropic = 58.8987 Anisotropy = 176.0403
XX= -6.4902 YX= 65.0117 ZX= 3.3478
XY= 65.8834 YY= 140.5995 ZY= -41.8860
XZ= 0.5216 YZ= -40.3288 ZZ= 42.5869
Eigenvalues: -35.2113 35.6486 176.2589
7 N Isotropic = 112.1593 Anisotropy = 91.8098
XX= 70.7920 YX= 37.1105 ZX= 14.2196
XY= 46.8107 YY= 148.8538 ZY= -29.9548
XZ= 25.7240 YZ= -25.7188 ZZ= 116.8322
Eigenvalues: 40.7570 122.3550 173.3659
8 C Isotropic = 59.0345 Anisotropy = 119.1122
XX= 51.7856 YX= 16.8194 ZX= -36.9083
XY= 23.7202 YY= 121.6263 ZY= -29.2085
XZ= -28.2093 YZ= -32.4864 ZZ= 3.6917
Eigenvalues: -15.4520 54.1129 138.4427
9 C Isotropic = 75.9268 Anisotropy = 106.1721
XX= 52.4192 YX= 20.2646 ZX= -32.0196
XY= 22.3402 YY= 134.4917 ZY= -18.9640
XZ= -36.3279 YZ= -18.2023 ZZ= 40.8693
Eigenvalues: 11.9842 69.0879 146.7082
10 C Isotropic = 19.7413 Anisotropy = 122.0836
XX= -12.3414 YX= 14.2179 ZX= -11.2173
XY= 20.0288 YY= 94.8090 ZY= 20.7467
XZ= -34.3251 YZ= 28.4464 ZZ= -23.2437
Eigenvalues: -47.4990 5.5925 101.1303
11 Br Isotropic = 1887.2488 Anisotropy = 1572.3951
XX= 1908.1943 YX= 40.6200 ZX= 731.8805
XY= 35.9490 YY= 1343.2413 ZY= 103.5582
XZ= 720.9067 YZ= 113.8099 ZZ= 2410.3109
Eigenvalues: 1321.0223 1405.2120 2935.5122
12 C Isotropic = 71.0123 Anisotropy = 87.2863
XX= 69.1828 YX= 9.0884 ZX= -4.3402

XY= 11.3558 YY= 121.6843 ZY= 25.8731
XZ= 6.3118 YZ= 23.5238 ZZ= 22.1698
Eigenvalues: 16.3407 67.4930 129.2031
 13 C Isotropic = 28.0509 Anisotropy = 77.4206
XX= -55.4907 YX= 18.8455 ZX= -43.3680
XY= 5.9466 YY= 78.5257 ZY= -0.3891
XZ= -12.4254 YZ= 5.8282 ZZ= 61.1177
Eigenvalues: -62.9592 67.4472 79.6646
 14 N Isotropic = -138.7347 Anisotropy = 277.0426
XX= -329.4568 YX= 41.5992 ZX= -4.6710
XY= 16.3645 YY= 33.1810 ZY= 57.4546
XZ= -2.4542 YZ= 26.7241 ZZ= -119.9282
Eigenvalues: -331.9870 -130.1774 45.9604
 15 O Isotropic = -77.2315 Anisotropy = 259.4455
XX= -110.0414 YX= 14.0983 ZX= 16.8789
XY= 33.4406 YY= 81.3637 ZY= 66.2991
XZ= 12.7982 YZ= 47.9144 ZZ= -203.0167
Eigenvalues: -215.0401 -112.3865 95.7322
 16 I Isotropic = 3739.2840 Anisotropy = 2047.6371
XX= 5086.3709 YX= -153.7457 ZX= 138.2534
XY= -92.8774 YY= 3325.2075 ZY= 137.3693
XZ= 168.0773 YZ= 31.8913 ZZ= 2806.2735
Eigenvalues: 2780.1027 3333.3738 5104.3754
 17 C Isotropic = 63.8301 Anisotropy = 109.1315
XX= 111.8385 YX= 31.9416 ZX= 15.9111
XY= 29.6494 YY= 54.5196 ZY= 44.5216
XZ= 19.8524 YZ= 42.2707 ZZ= 25.1323
Eigenvalues: -6.1022 61.0081 136.5845
 18 N Isotropic = 88.7327 Anisotropy = 127.7013
XX= 112.6068 YX= 70.2798 ZX= 48.2255
XY= 77.8556 YY= 60.5771 ZY= -19.4378
XZ= 33.9795 YZ= -8.8317 ZZ= 93.0143
Eigenvalues: -5.1168 97.4480 173.8669
 19 C Isotropic = 65.3595 Anisotropy = 120.0488
XX= 119.9296 YX= 28.4627 ZX= 23.7587
XY= 36.5798 YY= 63.9792 ZY= 37.2395
XZ= 17.9079 YZ= 45.6696 ZZ= 12.1696
Eigenvalues: -10.8606 61.5471 145.3920
 20 C Isotropic = 71.4321 Anisotropy = 139.4377
XX= 122.1228 YX= 43.6233 ZX= 45.3450
XY= 49.6592 YY= 78.7510 ZY= 5.3308
XZ= 50.9585 YZ= 3.0209 ZZ= 13.4225
Eigenvalues: -7.0563 56.9620 164.3906
 21 C Isotropic = 69.5722 Anisotropy = 141.6108
XX= 117.5421 YX= 63.6753 ZX= 21.8680
XY= 67.0744 YY= 31.0543 ZY= 33.6314
XZ= 22.4707 YZ= 27.4641 ZZ= 60.1203
Eigenvalues: -8.4698 53.2071 163.9794
 22 H Isotropic = 24.5291 Anisotropy = 11.9817
XX= 30.4609 YX= -1.6834 ZX= 4.1203
XY= -1.3489 YY= 19.2820 ZY= 1.4992
XZ= 4.1876 YZ= 0.9435 ZZ= 23.8444
Eigenvalues: 18.3477 22.7227 32.5169
 23 H Isotropic = 24.2282 Anisotropy = 9.6979
XX= 23.8571 YX= -1.4745 ZX= 1.0156
XY= -1.3758 YY= 19.1485 ZY= 3.2896
XZ= 0.5941 YZ= 3.4788 ZZ= 29.6789
Eigenvalues: 17.7386 24.2525 30.6935

24 H Isotropic = 25.0707 Anisotropy = 13.1149
XX= 30.5594 YX= 3.2447 ZX= 2.3924
XY= 3.7910 YY= 19.3960 ZY= 3.3082
XZ= 4.4834 YZ= 3.7221 ZZ= 25.2567
Eigenvalues: 17.4744 23.9237 33.8140
25 H Isotropic = 23.8087 Anisotropy = 9.5846
XX= 28.6981 YX= -4.0295 ZX= -0.3304
XY= -3.5715 YY= 17.5726 ZY= 2.2513
XZ= -0.6842 YZ= 2.8225 ZZ= 25.1553
Eigenvalues: 15.8368 25.3908 30.1984
26 H Isotropic = 23.9226 Anisotropy = 6.0116
XX= 26.6919 YX= -2.6037 ZX= -0.6574
XY= -3.4462 YY= 20.1721 ZY= 1.7588
XZ= 0.8644 YZ= 0.8594 ZZ= 24.9037
Eigenvalues: 18.7286 25.1089 27.9303
27 H Isotropic = 24.1974 Anisotropy = 3.5314
XX= 23.5878 YX= -2.6913 ZX= -2.3482
XY= -0.2243 YY= 25.1024 ZY= -1.7321
XZ= -3.1177 YZ= -0.3403 ZZ= 23.9020
Eigenvalues: 20.3464 25.6943 26.5517
28 H Isotropic = 25.0417 Anisotropy = 3.7047
XX= 24.3569 YX= -1.4676 ZX= -0.8107
XY= 0.4246 YY= 24.6386 ZY= -2.6010
XZ= -1.6294 YZ= -0.9874 ZZ= 26.1297
Eigenvalues: 22.6614 24.9523 27.5116
29 H Isotropic = 25.0907 Anisotropy = 2.8866
XX= 24.9716 YX= -1.7543 ZX= -1.0672
XY= -0.7518 YY= 23.8033 ZY= -1.1048
XZ= -0.9812 YZ= -0.3607 ZZ= 26.4974
Eigenvalues: 22.6440 25.6130 27.0152
30 H Isotropic = 24.9053 Anisotropy = 7.0141
XX= 23.6012 YX= -1.2021 ZX= 0.8911
XY= -2.1005 YY= 21.9181 ZY= 2.1827
XZ= 0.3997 YZ= 1.1884 ZZ= 29.1964
Eigenvalues: 20.5414 24.5931 29.5813

Isomer 7 (conformer 3)

1 C Isotropic = 56.3828 Anisotropy = 146.1923
XX= 34.9087 YX= 42.1909 ZX= 49.6346
XY= 42.1728 YY= 138.4358 ZY= -9.6435
XZ= 47.0070 YZ= -8.8781 ZZ= -4.1962
Eigenvalues: -42.4252 57.7293 153.8443
2 C Isotropic = 46.4192 Anisotropy = 115.1424
XX= 45.7230 YX= 31.8249 ZX= -40.2427
XY= 31.4492 YY= 109.8585 ZY= 22.9649
XZ= -36.4412 YZ= 22.2508 ZZ= -16.3238
Eigenvalues: -42.3969 58.4737 123.1808
3 C Isotropic = 70.2181 Anisotropy = 125.0603
XX= 13.1003 YX= 53.6968 ZX= -12.3154
XY= 54.4155 YY= 132.5352 ZY= 9.2200
XZ= -7.9971 YZ= 8.1077 ZZ= 65.0189
Eigenvalues: -9.8532 66.9159 153.5917
4 C Isotropic = 47.1825 Anisotropy = 139.6778
XX= 24.3303 YX= 42.1320 ZX= 31.5746
XY= 43.1131 YY= 124.1897 ZY= -3.9032
XZ= 30.1911 YZ= -3.0401 ZZ= -6.9723
Eigenvalues: -30.5493 31.7958 140.3011
5 C Isotropic = 59.2415 Anisotropy = 162.3275
XX= 28.7257 YX= 53.0872 ZX= -13.1744
XY= 52.1373 YY= 146.9833 ZY= 14.3641
XZ= -12.4408 YZ= 13.9113 ZZ= 2.0154
Eigenvalues: -12.2136 22.4781 167.4598
6 C Isotropic = 58.3947 Anisotropy = 172.0364
XX= -9.8712 YX= 68.2101 ZX= 13.8808
XY= 68.2223 YY= 147.1842 ZY= 2.9475
XZ= 9.1541 YZ= 4.3095 ZZ= 37.8711
Eigenvalues: -36.5842 38.6827 173.0856
7 N Isotropic = 112.4275 Anisotropy = 88.6839
XX= 60.4300 YX= 40.4483 ZX= 20.6715
XY= 32.5990 YY= 159.1268 ZY= 0.2116
XZ= 25.9885 YZ= -6.4991 ZZ= 117.7256
Eigenvalues: 41.3589 124.3735 171.5500
8 C Isotropic = 60.5049 Anisotropy = 122.8188
XX= 50.6831 YX= 34.3910 ZX= -18.1613
XY= 8.4221 YY= 136.9709 ZY= 8.8973
XZ= -11.8429 YZ= 13.6983 ZZ= -6.1392
Eigenvalues: -11.6640 50.7947 142.3841
9 C Isotropic = 75.9003 Anisotropy = 107.9827
XX= 61.0956 YX= 32.6983 ZX= -13.2431
XY= 32.9880 YY= 135.0125 ZY= 13.5357
XZ= -21.9079 YZ= 13.9822 ZZ= 31.5927
Eigenvalues: 16.9187 62.8934 147.8888
10 C Isotropic = 16.8571 Anisotropy = 123.6186
XX= -31.8497 YX= 44.5734 ZX= -4.6837
XY= 47.0938 YY= 83.1136 ZY= 1.6342
XZ= 21.3073 YZ= -0.1339 ZZ= -0.6927
Eigenvalues: -49.0807 0.3825 99.2694
11 Br Isotropic = 1891.3953 Anisotropy = 1571.8218
XX= 1651.7463 YX= -159.4243 ZX= 561.5420
XY= -153.5201 YY= 1398.5723 ZY= -280.4527
XZ= 539.1761 YZ= -284.2705 ZZ= 2623.8674
Eigenvalues: 1322.9993 1411.9102 2939.2765
12 C Isotropic = 73.3085 Anisotropy = 78.0775
XX= 50.2005 YX= 21.6822 ZX= 27.3803

XY= 18.8269 YY= 119.9001 ZY= -10.2711
XZ= 18.6634 YZ= -2.8360 ZZ= 49.8251
Eigenvalues: 23.2144 71.3510 125.3602
 13 C Isotropic = 28.6659 Anisotropy = 78.2875
XX= -3.3723 YX= 31.5740 ZX= -44.6372
XY= 41.5327 YY= 64.3288 ZY= 16.5110
XZ= -72.6196 YZ= 28.0535 ZZ= 25.0413
Eigenvalues: -63.6317 68.7718 80.8576
 14 N Isotropic = -133.3394 Anisotropy = 267.3167
XX= -193.6144 YX= 82.4557 ZX= -73.4150
XY= 93.5608 YY= 10.9696 ZY= 53.4005
XZ= -93.0744 YZ= 44.4917 ZZ= -217.3732
Eigenvalues: -317.3731 -127.5167 44.8718
 15 O Isotropic = -77.1013 Anisotropy = 273.1659
XX= -144.6269 YX= 80.1806 ZX= 54.1688
XY= 83.8706 YY= 76.0111 ZY= 10.0632
XZ= 54.9962 YZ= -0.1790 ZZ= -162.6880
Eigenvalues: -218.3837 -117.9294 105.0093
 16 I Isotropic = 3774.4194 Anisotropy = 2031.8345
XX= 3872.9238 YX= -224.3543 ZX= 1086.7881
XY= -263.2360 YY= 3456.1593 ZY= -437.0666
XZ= 1029.8320 YZ= -409.3420 ZZ= 3994.1750
Eigenvalues: 2847.9756 3346.3068 5128.9757
 17 C Isotropic = 63.2100 Anisotropy = 108.7600
XX= 86.2910 YX= -31.3063 ZX= 17.4037
XY= -26.5493 YY= 89.9819 ZY= -46.9170
XZ= 23.1086 YZ= -44.0074 ZZ= 13.3571
Eigenvalues: -8.2345 62.1478 135.7167
 18 N Isotropic = 86.5384 Anisotropy = 126.2066
XX= 54.6041 YX= -79.0160 ZX= 18.2094
XY= -76.9964 YY= 104.0192 ZY= -19.0573
XZ= 11.3787 YZ= -23.1860 ZZ= 100.9919
Eigenvalues: -2.5169 91.4560 170.6761
 19 C Isotropic = 65.0963 Anisotropy = 118.8303
XX= 88.4841 YX= -26.5644 ZX= 33.8752
XY= -35.1219 YY= 96.9698 ZY= -41.7908
XZ= 24.1612 YZ= -46.4611 ZZ= 9.8350
Eigenvalues: -11.1463 62.1187 144.3165
 20 C Isotropic = 72.7995 Anisotropy = 136.7069
XX= 64.4696 YX= -50.3194 ZX= 51.3268
XY= -52.8999 YY= 113.4060 ZY= -21.0374
XZ= 56.6547 YZ= -17.4953 ZZ= 40.5229
Eigenvalues: -5.9386 60.3997 163.9375
 21 C Isotropic = 71.6299 Anisotropy = 137.8428
XX= 77.1818 YX= -63.7573 ZX= 0.5143
XY= -61.5860 YY= 87.1613 ZY= -64.2353
XZ= 7.8832 YZ= -47.6832 ZZ= 50.5466
Eigenvalues: -7.5069 58.8715 163.5251
 22 H Isotropic = 24.0509 Anisotropy = 10.0471
XX= 27.3004 YX= -3.5642 ZX= 2.8586
XY= -3.5652 YY= 19.5991 ZY= -1.5075
XZ= 3.1495 YZ= -1.5538 ZZ= 25.2533
Eigenvalues: 18.1844 23.2195 30.7490
 23 H Isotropic = 24.1907 Anisotropy = 10.2902
XX= 23.1327 YX= -1.9362 ZX= -0.5343
XY= -1.9561 YY= 18.4951 ZY= -0.6804
XZ= -1.2586 YZ= -0.2561 ZZ= 30.9443
Eigenvalues: 17.7442 23.7771 31.0508

24 H Isotropic = 22.9788 Anisotropy = 10.3663
XX= 22.5632 YX= -2.3347 ZX= 1.7728
XY= -2.2818 YY= 16.9849 ZY= -1.3151
XZ= 1.1155 YZ= -1.0239 ZZ= 29.3882
Eigenvalues: 16.1246 22.9221 29.8896
25 H Isotropic = 24.0145 Anisotropy = 8.9800
XX= 28.0710 YX= -4.5376 ZX= 0.1088
XY= -5.2336 YY= 17.6149 ZY= -0.9436
XZ= -0.7962 YZ= -0.2564 ZZ= 26.3576
Eigenvalues: 15.6437 26.3986 30.0012
26 H Isotropic = 23.5238 Anisotropy = 12.4607
XX= 26.6733 YX= -3.4596 ZX= 2.8292
XY= -2.6609 YY= 16.7915 ZY= -4.6076
XZ= 4.0123 YZ= -2.7296 ZZ= 27.1065
Eigenvalues: 15.2704 23.4701 31.8309
27 H Isotropic = 23.7413 Anisotropy = 5.1018
XX= 25.2965 YX= 0.8187 ZX= -1.7100
XY= 1.5221 YY= 22.9204 ZY= 4.9902
XZ= -2.1461 YZ= 2.8892 ZZ= 23.0070
Eigenvalues: 18.3328 25.7485 27.1425
28 H Isotropic = 24.6317 Anisotropy = 3.9325
XX= 24.8933 YX= 1.3438 ZX= -0.6591
XY= 0.5701 YY= 22.7583 ZY= 2.1348
XZ= -1.7524 YZ= 1.3870 ZZ= 26.2434
Eigenvalues: 21.4761 25.1656 27.2533
29 H Isotropic = 25.1112 Anisotropy = 2.8519
XX= 25.7310 YX= 1.2175 ZX= -0.9928
XY= 0.9458 YY= 23.4320 ZY= 0.5488
XZ= -1.0571 YZ= 0.6958 ZZ= 26.1706
Eigenvalues: 22.7254 25.5957 27.0124
30 H Isotropic = 24.9861 Anisotropy = 5.1263
XX= 25.8619 YX= 0.6759 ZX= -1.9451
XY= 1.4021 YY= 22.6190 ZY= -2.1791
XZ= -1.3743 YZ= -0.7140 ZZ= 26.4775
Eigenvalues: 22.0673 24.4874 28.4037

Isomer 7 (conformer 4)

1 C Isotropic = 57.4657 Anisotropy = 143.8626
XX= 59.2650 YX= 50.9657 ZX= 24.0493
XY= 51.2605 YY= 112.9751 ZY= -55.9942
XZ= 22.2244 YZ= -55.4976 ZZ= 0.1569
Eigenvalues: -40.8975 59.9205 153.3741
2 C Isotropic = 46.9537 Anisotropy = 114.0644
XX= 31.5348 YX= 23.8776 ZX= -58.3070
XY= 24.0471 YY= 108.5501 ZY= -12.6087
XZ= -52.8434 YZ= -12.0302 ZZ= 0.7762
Eigenvalues: -41.6621 59.5265 122.9966
3 C Isotropic = 70.5658 Anisotropy = 124.5152
XX= 14.9090 YX= 55.2574 ZX= -16.3714
XY= 55.1323 YY= 124.9903 ZY= -16.4112
XZ= -11.6512 YZ= -18.5506 ZZ= 71.7981
Eigenvalues: -8.5022 66.6237 153.5760
4 C Isotropic = 46.5942 Anisotropy = 139.1142
XX= 36.7600 YX= 46.1296 ZX= 9.0632
XY= 45.6737 YY= 106.6089 ZY= -47.5261
XZ= 10.0246 YZ= -44.2284 ZZ= -3.5863
Eigenvalues: -30.7631 31.2087 139.3370
5 C Isotropic = 60.3818 Anisotropy = 163.8129
XX= 28.1753 YX= 53.0823 ZX= -32.0793
XY= 52.4516 YY= 138.4051 ZY= -26.5375
XZ= -32.4987 YZ= -31.7660 ZZ= 14.5651
Eigenvalues: -12.7671 24.3222 169.5904
6 C Isotropic = 59.2020 Anisotropy = 175.3782
XX= 8.0547 YX= 80.2854 ZX= 1.8537
XY= 79.0979 YY= 128.2900 ZY= -35.4022
XZ= -1.9769 YZ= -38.1451 ZZ= 41.2613
Eigenvalues: -35.3975 36.8828 176.1208
7 N Isotropic = 112.6326 Anisotropy = 91.1548
XX= 79.8720 YX= 43.7091 ZX= 11.8748
XY= 51.8458 YY= 141.8928 ZY= -30.2082
XZ= 24.6171 YZ= -27.4991 ZZ= 116.1329
Eigenvalues: 41.6369 122.8584 173.4024
8 C Isotropic = 59.0576 Anisotropy = 119.3283
XX= 57.1516 YX= 24.5904 ZX= -39.3266
XY= 32.3951 YY= 117.8367 ZY= -21.6093
XZ= -30.0852 YZ= -26.6244 ZZ= 2.1845
Eigenvalues: -15.3324 53.8954 138.6098
9 C Isotropic = 75.6676 Anisotropy = 107.1401
XX= 56.8777 YX= 29.3282 ZX= -32.6087
XY= 30.9066 YY= 130.8943 ZY= -12.8727
XZ= -37.2519 YZ= -11.9630 ZZ= 39.2308
Eigenvalues: 11.3116 68.5969 147.0943
10 C Isotropic = 17.2802 Anisotropy = 125.6003
XX= -10.1924 YX= 23.9244 ZX= -8.8122
XY= 34.0899 YY= 86.3378 ZY= 30.4477
XZ= -30.6777 YZ= 38.7106 ZZ= -24.3047
Eigenvalues: -52.7825 3.6094 101.0138
11 Br Isotropic = 1891.6251 Anisotropy = 1576.2469
XX= 1895.8793 YX= -44.1000 ZX= 732.2491
XY= -36.1058 YY= 1339.8716 ZY= 2.6965
XZ= 718.8816 YZ= 7.9310 ZZ= 2439.1245
Eigenvalues: 1321.4929 1410.9261 2942.4564
12 C Isotropic = 70.5732 Anisotropy = 84.5526
XX= 73.0642 YX= 12.0833 ZX= 0.6633

XY= 13.7075 YY= 114.6291 ZY= 31.2768
XZ= 9.9833 YZ= 27.6450 ZZ= 24.0263
Eigenvalues: 15.2523 69.5258 126.9416
 13 C Isotropic = 28.6550 Anisotropy = 78.9564
XX= -54.8986 YX= 33.7878 ZX= -38.5433
XY= 18.0921 YY= 76.2404 ZY= 5.7360
XZ= -9.6816 YZ= 5.8012 ZZ= 64.6233
Eigenvalues: -64.5904 69.2629 81.2926
 14 N Isotropic = -138.6832 Anisotropy = 276.0358
XX= -319.7017 YX= 71.6757 ZX= 4.9320
XY= 46.2188 YY= 18.4577 ZY= 69.3747
XZ= 5.7959 YZ= 34.3335 ZZ= -114.8057
Eigenvalues: -329.7374 -131.6529 45.3406
 15 O Isotropic = -81.2277 Anisotropy = 262.6149
XX= -109.5859 YX= 29.9593 ZX= 22.1418
XY= 51.9626 YY= 64.8354 ZY= 84.5224
XZ= 16.7707 YZ= 63.0942 ZZ= -198.9326
Eigenvalues: -218.8827 -118.6493 93.8489
 16 I Isotropic = 3788.8691 Anisotropy = 2036.4075
XX= 5090.7575 YX= -329.8923 ZX= 10.2039
XY= -296.7833 YY= 3382.4244 ZY= 141.5020
XZ= 50.9723 YZ= 71.8798 ZZ= 2893.4254
Eigenvalues: 2866.8678 3353.2654 5146.4741
 17 C Isotropic = 64.3449 Anisotropy = 110.0356
XX= 112.1795 YX= 23.1411 ZX= 49.5870
XY= 25.7278 YY= 62.0938 ZY= -14.6770
XZ= 48.3758 YZ= -6.9400 ZZ= 18.7613
Eigenvalues: -7.8674 63.2001 137.7019
 18 N Isotropic = 88.3100 Anisotropy = 126.3170
XX= 155.3600 YX= 34.2558 ZX= 18.4652
XY= 36.9720 YY= 6.8059 ZY= 30.8893
XZ= 20.4249 YZ= 20.7898 ZZ= 102.7641
Eigenvalues: -5.4605 97.8691 172.5213
 19 C Isotropic = 65.3764 Anisotropy = 119.2236
XX= 123.7348 YX= 17.3244 ZX= 44.5191
XY= 22.6338 YY= 63.6665 ZY= -0.8787
XZ= 52.4914 YZ= -12.3367 ZZ= 8.7280
Eigenvalues: -11.3286 62.5990 144.8589
 20 C Isotropic = 71.8168 Anisotropy = 139.9848
XX= 146.2079 YX= 17.0255 ZX= 39.9950
XY= 22.1174 YY= 45.2787 ZY= 35.7475
XZ= 38.1017 YZ= 38.9690 ZZ= 23.9639
Eigenvalues: -7.0262 57.3367 165.1400
 21 C Isotropic = 68.6206 Anisotropy = 142.3038
XX= 134.3181 YX= 44.6331 ZX= 46.0618
XY= 49.1827 YY= 16.4257 ZY= -18.1990
XZ= 41.1139 YZ= -10.6625 ZZ= 55.1180
Eigenvalues: -13.0158 55.3878 163.4898
 22 H Isotropic = 24.5684 Anisotropy = 12.0827
XX= 30.0062 YX= -2.8671 ZX= 4.2610
XY= -2.7573 YY= 19.6401 ZY= 0.8431
XZ= 4.2773 YZ= 0.3444 ZZ= 24.0588
Eigenvalues: 18.3312 22.7505 32.6235
 23 H Isotropic = 24.2269 Anisotropy = 9.6850
XX= 23.5383 YX= -1.9996 ZX= 1.1976
XY= -1.9093 YY= 19.2761 ZY= 2.8452
XZ= 0.8342 YZ= 3.1206 ZZ= 29.8661
Eigenvalues: 17.7007 24.2963 30.6835

24 H Isotropic = 25.3162 Anisotropy = 12.7066
XX= 31.2505 YX= 2.1393 ZX= 2.8549
XY= 1.3042 YY= 18.6794 ZY= 2.2352
XZ= 4.8768 YZ= 2.7477 ZZ= 26.0187
Eigenvalues: 17.8907 24.2706 33.7872
25 H Isotropic = 23.8468 Anisotropy = 9.6831
XX= 27.8759 YX= -5.0851 ZX= -0.2537
XY= -4.7759 YY= 18.3949 ZY= 2.0821
XZ= -0.4423 YZ= 2.6379 ZZ= 25.2696
Eigenvalues: 15.8508 25.3874 30.3022
26 H Isotropic = 23.9436 Anisotropy = 5.9755
XX= 26.0342 YX= -3.1220 ZX= -0.5793
XY= -4.0158 YY= 20.8311 ZY= 1.7863
XZ= 0.7775 YZ= 0.6734 ZZ= 24.9655
Eigenvalues: 18.8040 25.0995 27.9273
27 H Isotropic = 23.6561 Anisotropy = 4.9593
XX= 19.4764 YX= -2.2624 ZX= 1.3441
XY= -3.5171 YY= 24.6589 ZY= 0.9621
XZ= 0.5775 YZ= -0.0528 ZZ= 26.8331
Eigenvalues: 18.0575 25.9485 26.9623
28 H Isotropic = 24.5619 Anisotropy = 3.8570
XX= 23.4296 YX= -1.7236 ZX= -1.9442
XY= -1.1862 YY= 23.7913 ZY= 0.2856
XZ= -1.1076 YZ= -0.8215 ZZ= 26.4650
Eigenvalues: 21.7574 24.7951 27.1333
29 H Isotropic = 25.2985 Anisotropy = 2.8724
XX= 24.4763 YX= -0.7159 ZX= -1.1879
XY= 0.4406 YY= 25.2919 ZY= -1.1781
XZ= -1.2171 YZ= -1.0099 ZZ= 26.1272
Eigenvalues: 23.5710 25.1110 27.2134
30 H Isotropic = 25.5429 Anisotropy = 4.6436
XX= 25.2856 YX= 0.4153 ZX= -0.8131
XY= 2.4975 YY= 26.0282 ZY= -2.6578
XZ= -1.2755 YZ= -1.3053 ZZ= 25.3148
Eigenvalues: 23.6375 24.3526 28.6386

Isomer 8 (conformer 1)

1 C Isotropic = 58.3545 Anisotropy = 144.7060
XX= 44.8443 YX= -30.7937 ZX= 34.5001
XY= -27.9153 YY= 2.6514 ZY= 57.9819
XZ= 33.8013 YZ= 58.3029 ZZ= 127.5678
Eigenvalues: -39.5445 59.7828 154.8251
2 C Isotropic = 46.9367 Anisotropy = 113.6135
XX= 18.5673 YX= 55.6490 ZX= 3.8535
XY= 52.0646 YY= 9.9616 ZY= 26.9342
XZ= 5.3390 YZ= 27.1365 ZZ= 112.2811
Eigenvalues: -41.6380 59.7690 122.6790
3 C Isotropic = 70.4409 Anisotropy = 124.6606
XX= -1.7580 YX= 10.3129 ZX= 29.8499
XY= 4.8780 YY= 75.2145 ZY= 25.7741
XZ= 32.8315 YZ= 25.1793 ZZ= 137.8662
Eigenvalues: -8.5254 66.3002 153.5480
4 C Isotropic = 47.0199 Anisotropy = 143.2893
XX= 22.8382 YX= -12.2585 ZX= 29.5287
XY= -13.2098 YY= 1.7453 ZY= 52.6703
XZ= 29.5553 YZ= 55.9616 ZZ= 116.4763
Eigenvalues: -30.2480 28.7616 142.5461
5 C Isotropic = 57.3192 Anisotropy = 168.9483
XX= 2.1730 YX= 22.8589 ZX= 26.7543
XY= 19.5768 YY= 22.9167 ZY= 48.2816
XZ= 29.1114 YZ= 47.8199 ZZ= 146.8680
Eigenvalues: -11.1054 13.1117 169.9514
6 C Isotropic = 60.3631 Anisotropy = 173.6876
XX= -21.0810 YX= -10.1793 ZX= 46.4156
XY= -9.5616 YY= 50.6508 ZY= 44.4933
XZ= 46.7948 YZ= 42.7062 ZZ= 151.5194
Eigenvalues: -37.9443 42.8787 176.1548
7 N Isotropic = 116.5739 Anisotropy = 86.1081
XX= 73.3101 YX= -20.6578 ZX= 28.1529
XY= -28.1447 YY= 120.9078 ZY= 26.0362
XZ= 34.8737 YZ= 29.5424 ZZ= 155.5038
Eigenvalues: 47.9681 127.7742 173.9793
8 C Isotropic = 59.6617 Anisotropy = 115.3732
XX= 44.6727 YX= 41.3075 ZX= 2.9991
XY= 33.6209 YY= 12.1554 ZY= 38.5929
XZ= 7.6905 YZ= 35.5360 ZZ= 122.1571
Eigenvalues: -18.3246 60.7325 136.5772
9 C Isotropic = 75.0532 Anisotropy = 112.7974
XX= 31.4469 YX= 33.3782 ZX= 12.3197
XY= 40.3041 YY= 55.2062 ZY= 26.2501
XZ= 8.6684 YZ= 27.3949 ZZ= 138.5066
Eigenvalues: 4.1880 70.7202 150.2515
10 C Isotropic = 65.9641 Anisotropy = 94.6635
XX= -8.5929 YX= -4.0225 ZX= -16.4753
XY= -3.4268 YY= 98.9395 ZY= -27.0885
XZ= -15.8736 YZ= -22.3441 ZZ= 107.5457
Eigenvalues: -11.2730 80.0922 129.0731
11 Br Isotropic = 1882.1482 Anisotropy = 1560.9063
XX= 1979.8534 YX= -743.2101 ZX= 106.5723
XY= -714.5272 YY= 2308.5038 ZY= -182.4857
XZ= 125.1311 YZ= -199.8469 ZZ= 1358.0873
Eigenvalues: 1316.5098 1407.1823 2922.7524
12 C Isotropic = 26.4583 Anisotropy = 145.2502
XX= 13.1655 YX= -5.5354 ZX= -15.8675

XY= -27.1080 YY= 28.3586 ZY= -89.7544
XZ= -32.8748 YZ= -89.5804 ZZ= 37.8509
Eigenvalues: -66.9373 23.0206 123.2918
13 N Isotropic = -143.6943 Anisotropy = 254.0640
XX= -150.7621 YX= 30.1290 ZX= 8.7727
XY= 22.4540 YY= -157.3461 ZY= -165.4898
XZ= 5.2277 YZ= -162.6401 ZZ= -122.9747
Eigenvalues: -308.8447 -147.9199 25.6817
14 O Isotropic = -61.1820 Anisotropy = 245.6330
XX= -136.9377 YX= 34.5724 ZX= 5.9088
XY= 50.2905 YY= -28.3598 ZY= -117.1336
XZ= -0.3051 YZ= -128.0501 ZZ= -18.2486
Eigenvalues: -175.5395 -110.5799 102.5733
15 C Isotropic = 28.7583 Anisotropy = 69.3908
XX= 17.9661 YX= -43.3841 ZX= -50.5576
XY= -41.4758 YY= 43.2028 ZY= -22.3964
XZ= -28.3549 YZ= -31.4306 ZZ= 25.1060
Eigenvalues: -45.8077 57.0637 75.0188
16 I Isotropic = 3656.5430 Anisotropy = 2183.7342
XX= 3173.2574 YX= 682.7819 ZX= 744.1636
XY= 803.1955 YY= 3791.8017 ZY= 597.3077
XZ= 721.9072 YZ= 696.2093 ZZ= 4004.5700
Eigenvalues: 2605.2187 3252.0446 5112.3658
17 C Isotropic = 61.8802 Anisotropy = 105.1266
XX= 34.0106 YX= -24.3180 ZX= -15.6316
XY= -17.1455 YY= 73.6638 ZY= -55.2313
XZ= -7.5024 YZ= -56.2028 ZZ= 77.9662
Eigenvalues: 2.9365 50.7395 131.9646
18 N Isotropic = 98.5349 Anisotropy = 127.5491
XX= 24.4929 YX= 20.3519 ZX= 32.7632
XY= 15.4223 YY= 132.9585 ZY= -50.7811
XZ= 28.7789 YZ= -43.7237 ZZ= 138.1533
Eigenvalues: 9.1669 102.8702 183.5676
19 C Isotropic = 63.7038 Anisotropy = 118.8181
XX= 47.2375 YX= -21.8270 ZX= -13.7845
XY= -29.7193 YY= 69.3216 ZY= -70.0457
XZ= -17.2122 YZ= -70.8063 ZZ= 74.5522
Eigenvalues: -12.8963 61.0918 142.9158
20 C Isotropic = 72.5834 Anisotropy = 134.1783
XX= 55.7008 YX= 8.8883 ZX= 17.3423
XY= 10.9525 YY= 80.8805 ZY= -80.4218
XZ= 20.9996 YZ= -80.7701 ZZ= 81.1688
Eigenvalues: -6.4087 62.1233 162.0356
21 C Isotropic = 68.3261 Anisotropy = 147.5340
XX= -6.9002 YX= -11.4642 ZX= 3.1500
XY= -8.9557 YY= 100.2049 ZY= -62.9497
XZ= 6.1672 YZ= -56.7610 ZZ= 111.6737
Eigenvalues: -7.8762 46.1724 166.6822
22 H Isotropic = 24.3929 Anisotropy = 9.7619
XX= 29.3705 YX= -2.7380 ZX= -1.2465
XY= -3.6436 YY= 24.2355 ZY= -1.5148
XZ= -0.6177 YZ= -1.6450 ZZ= 19.5726
Eigenvalues: 18.7307 23.5471 30.9008
23 H Isotropic = 24.1191 Anisotropy = 9.8600
XX= 23.7925 YX= -1.3292 ZX= -0.8614
XY= -1.0032 YY= 29.4412 ZY= -3.6570
XZ= -0.7076 YZ= -3.5656 ZZ= 19.1238
Eigenvalues: 17.7824 23.8825 30.6925

24 H Isotropic = 24.2555 Anisotropy = 9.5483
XX= 23.5945 YX= -2.0995 ZX= 0.4044
XY= -3.2776 YY= 28.1395 ZY= -3.5726
XZ= 1.7212 YZ= -3.0158 ZZ= 21.0324
Eigenvalues: 19.7404 22.4050 30.6210
25 H Isotropic = 23.8120 Anisotropy = 9.6165
XX= 29.0528 YX= 0.1492 ZX= -3.2006
XY= 0.8675 YY= 24.6385 ZY= -2.8015
XZ= -3.4106 YZ= -2.5349 ZZ= 17.7447
Eigenvalues: 16.1389 25.0741 30.2230
26 H Isotropic = 24.5032 Anisotropy = 6.3643
XX= 26.4861 YX= 0.7842 ZX= -3.3027
XY= -0.4361 YY= 24.3820 ZY= -0.2258
XZ= -3.9118 YZ= -1.6753 ZZ= 22.6415
Eigenvalues: 20.3444 24.4192 28.7461
27 H Isotropic = 22.9282 Anisotropy = 7.7548
XX= 27.5928 YX= -0.6251 ZX= -0.9816
XY= -0.4105 YY= 20.9799 ZY= 5.3239
XZ= -1.0413 YZ= 5.0310 ZZ= 20.2120
Eigenvalues: 15.3918 25.2948 28.0981
28 H Isotropic = 24.7887 Anisotropy = 3.7975
XX= 26.4176 YX= 0.9507 ZX= 0.8450
XY= 0.0616 YY= 23.9542 ZY= 2.5057
XZ= 0.5758 YZ= 2.5384 ZZ= 23.9941
Eigenvalues: 21.4479 25.5977 27.3203
29 H Isotropic = 25.5727 Anisotropy = 4.2539
XX= 26.6850 YX= 0.7006 ZX= 0.8671
XY= 0.4432 YY= 24.4453 ZY= 2.2630
XZ= 1.4633 YZ= 2.5034 ZZ= 25.5878
Eigenvalues: 22.5463 25.7632 28.4086
30 H Isotropic = 25.7902 Anisotropy = 11.8114
XX= 25.3592 YX= 0.1934 ZX= 2.4324
XY= 2.2112 YY= 23.5711 ZY= 4.8535
XZ= 6.6831 YZ= 4.2211 ZZ= 28.4403
Eigenvalues: 20.3138 23.3924 33.6645

Isomer 8 (conformer 2)

1 C Isotropic = 57.4839 Anisotropy = 146.4771
XX= 37.3972 YX= -37.7207 ZX= 29.3178
XY= -35.0075 YY= -3.7623 ZY= 45.5450
XZ= 29.1357 YZ= 45.6754 ZZ= 138.8169
Eigenvalues: -41.2398 58.5563 155.1353
2 C Isotropic = 46.6726 Anisotropy = 114.8907
XX= 20.7129 YX= 53.5552 ZX= 3.5015
XY= 49.3529 YY= 2.6695 ZY= 22.2800
XZ= 4.9950 YZ= 22.9271 ZZ= 116.6353
Eigenvalues: -41.9136 58.6649 123.2664
3 C Isotropic = 70.4502 Anisotropy = 124.6508
XX= -4.2816 YX= 10.2398 ZX= 23.4892
XY= 4.0404 YY= 71.3108 ZY= 20.3600
XZ= 25.4888 YZ= 19.6044 ZZ= 144.3213
Eigenvalues: -8.4091 66.2089 153.5507
4 C Isotropic = 47.0653 Anisotropy = 142.6167
XX= 19.6209 YX= -17.2762 ZX= 24.1512
XY= -18.4977 YY= -4.5926 ZY= 41.7490
XZ= 24.9693 YZ= 45.2446 ZZ= 126.1676
Eigenvalues: -30.0494 29.1021 142.1431
5 C Isotropic = 57.6651 Anisotropy = 167.3280
XX= 2.6330 YX= 19.6292 ZX= 22.3466
XY= 17.3698 YY= 15.7664 ZY= 37.3610
XZ= 26.3759 YZ= 39.0634 ZZ= 154.5958
Eigenvalues: -10.4714 14.2495 169.2171
6 C Isotropic = 60.4354 Anisotropy = 174.7599
XX= -26.1214 YX= -13.3296 ZX= 37.0725
XY= -12.8097 YY= 44.7219 ZY= 34.4437
XZ= 37.1485 YZ= 32.9217 ZZ= 162.7057
Eigenvalues: -37.8341 42.1983 176.9420
7 N Isotropic = 116.0683 Anisotropy = 86.9426
XX= 67.5557 YX= -21.0720 ZX= 22.3477
XY= -29.7176 YY= 118.6623 ZY= 20.8039
XZ= 29.2405 YZ= 25.3075 ZZ= 161.9867
Eigenvalues: 47.6352 126.5395 174.0300
8 C Isotropic = 59.1774 Anisotropy = 116.6617
XX= 46.1992 YX= 36.3565 ZX= 3.2710
XY= 30.4776 YY= 4.0454 ZY= 32.2974
XZ= 6.8773 YZ= 31.2354 ZZ= 127.2877
Eigenvalues: -18.9321 59.5126 136.9519
9 C Isotropic = 76.3413 Anisotropy = 111.6183
XX= 35.7856 YX= 31.4679 ZX= 10.0307
XY= 38.0188 YY= 50.0356 ZY= 21.3920
XZ= 7.9326 YZ= 22.8951 ZZ= 143.2028
Eigenvalues: 7.0598 71.2107 150.7535
10 C Isotropic = 66.9939 Anisotropy = 95.1390
XX= -6.4749 YX= -2.8281 ZX= -18.2109
XY= 1.4814 YY= 96.9005 ZY= -27.2653
XZ= -22.7389 YZ= -20.3963 ZZ= 110.5560
Eigenvalues: -10.1648 80.7265 130.4199
11 Br Isotropic = 1875.8882 Anisotropy = 1568.8313
XX= 1914.6231 YX= -728.7107 ZX= 85.8957
XY= -710.2031 YY= 2378.2929 ZY= -155.1391
XZ= 86.5284 YZ= -153.7270 ZZ= 1334.7488
Eigenvalues: 1309.8037 1396.0853 2921.7757
12 C Isotropic = 26.2497 Anisotropy = 143.7296
XX= 14.7852 YX= -5.1741 ZX= -15.9847

XY= -26.4807 YY= 19.3518 ZY= -88.1795
XZ= -33.0829 YZ= -88.9084 ZZ= 44.6123
Eigenvalues: -67.0967 23.7764 122.0695
13 N Isotropic = -158.4902 Anisotropy = 270.9976
XX= -158.7665 YX= 34.6675 ZX= 3.0972
XY= 22.4229 YY= -197.8496 ZY= -182.5497
XZ= 5.9572 YZ= -167.4208 ZZ= -118.8544
Eigenvalues: -341.2098 -156.4356 22.1749
14 O Isotropic = -71.6808 Anisotropy = 258.6864
XX= -152.4385 YX= 41.7468 ZX= -0.6805
XY= 68.6983 YY= -46.3980 ZY= -117.3826
XZ= -15.7432 YZ= -130.2093 ZZ= -16.2059
Eigenvalues: -193.3419 -122.4773 100.7767
15 C Isotropic = 30.2965 Anisotropy = 70.4916
XX= 23.6996 YX= -43.7567 ZX= -48.3618
XY= -42.5811 YY= 42.5082 ZY= -24.1519
XZ= -24.2362 YZ= -35.3434 ZZ= 24.6818
Eigenvalues: -43.4185 57.0171 77.2909
16 I Isotropic = 3667.1856 Anisotropy = 2196.2032
XX= 3111.6506 YX= 679.9246 ZX= 709.3107
XY= 782.1882 YY= 3814.6330 ZY= 584.7195
XZ= 705.4767 YZ= 747.4807 ZZ= 4075.2732
Eigenvalues: 2589.8400 3280.3958 5131.3211
17 C Isotropic = 62.7760 Anisotropy = 104.0026
XX= 54.6360 YX= 4.4034 ZX= 40.4092
XY= 2.9669 YY= 66.8207 ZY= -55.5184
XZ= 39.2399 YZ= -56.2538 ZZ= 66.8713
Eigenvalues: -6.0531 62.2701 132.1110
18 N Isotropic = 92.4350 Anisotropy = 140.2552
XX= 24.0026 YX= -50.6523 ZX= 30.0760
XY= -38.3189 YY= 110.9068 ZY= -42.7373
XZ= 34.4832 YZ= -36.0845 ZZ= 142.3957
Eigenvalues: 3.5274 87.8392 185.9385
19 C Isotropic = 64.0730 Anisotropy = 119.3954
XX= 64.8243 YX= -5.9922 ZX= 31.3252
XY= 1.9725 YY= 60.8594 ZY= -70.3132
XZ= 40.8782 YZ= -69.4880 ZZ= 66.5351
Eigenvalues: -13.8068 62.3558 143.6699
20 C Isotropic = 71.9480 Anisotropy = 137.8882
XX= 58.9118 YX= -42.1229 ZX= 12.6176
XY= -46.4872 YY= 57.1240 ZY= -68.7911
XZ= 15.5144 YZ= -67.3187 ZZ= 99.8081
Eigenvalues: -6.2247 58.1952 163.8734
21 C Isotropic = 70.9576 Anisotropy = 140.1044
XX= 21.9145 YX= -16.8833 ZX= 53.3342
XY= -23.1968 YY= 88.0953 ZY= -53.0619
XZ= 53.5355 YZ= -42.2579 ZZ= 102.8628
Eigenvalues: -4.7906 53.3028 164.3605
22 H Isotropic = 24.4619 Anisotropy = 10.0788
XX= 29.5193 YX= -2.8880 ZX= -0.6062
XY= -3.7090 YY= 24.5706 ZY= -1.4270
XZ= -0.0744 YZ= -1.6531 ZZ= 19.2958
Eigenvalues: 18.7262 23.4784 31.1811
23 H Isotropic = 24.1370 Anisotropy = 9.8457
XX= 24.0266 YX= -0.8512 ZX= -0.7861
XY= -0.6192 YY= 29.9753 ZY= -2.9204
XZ= -0.6137 YZ= -2.8460 ZZ= 18.4091
Eigenvalues: 17.6171 24.0930 30.7008

24 H Isotropic = 24.4851 Anisotropy = 9.2524
XX= 23.8829 YX= -1.6263 ZX= 1.4072
XY= -2.9706 YY= 28.1075 ZY= -3.7418
XZ= 2.2670 YZ= -2.8449 ZZ= 21.4650
Eigenvalues: 19.8939 22.9081 30.6534
25 H Isotropic = 23.7165 Anisotropy = 9.6157
XX= 29.3789 YX= 0.4608 ZX= -2.6236
XY= 0.9867 YY= 25.0484 ZY= -2.1409
XZ= -2.5477 YZ= -1.7014 ZZ= 16.7222
Eigenvalues: 15.8790 25.1435 30.1269
26 H Isotropic = 24.3019 Anisotropy = 6.7533
XX= 26.8140 YX= 0.7273 ZX= -3.3499
XY= -0.6633 YY= 24.2935 ZY= 0.3227
XZ= -4.1051 YZ= -0.8653 ZZ= 21.7981
Eigenvalues: 19.8021 24.2994 28.8041
27 H Isotropic = 24.1967 Anisotropy = 11.9924
XX= 26.4563 YX= 3.0376 ZX= 0.7812
XY= 4.9188 YY= 21.0465 ZY= 5.3385
XZ= 5.0069 YZ= 4.4061 ZZ= 25.0874
Eigenvalues: 17.3863 23.0121 32.1917
28 H Isotropic = 25.2402 Anisotropy = 4.8313
XX= 25.6881 YX= 0.5091 ZX= -0.4603
XY= 1.5254 YY= 24.3136 ZY= 2.6053
XZ= 1.6194 YZ= 3.2601 ZZ= 25.7187
Eigenvalues: 21.9460 25.3135 28.4610
29 H Isotropic = 25.2750 Anisotropy = 3.0175
XX= 26.3828 YX= 0.7298 ZX= -0.4920
XY= 1.0180 YY= 24.7549 ZY= 1.6801
XZ= 0.7318 YZ= 2.2632 ZZ= 24.6873
Eigenvalues: 22.6717 25.8666 27.2866
30 H Isotropic = 24.4481 Anisotropy = 4.2148
XX= 25.4307 YX= 1.0716 ZX= 0.1553
XY= 1.5001 YY= 25.2301 ZY= 2.9317
XZ= -0.4792 YZ= 1.8221 ZZ= 22.6836
Eigenvalues: 21.1059 24.9805 27.2580

Isomer 8 (conformer 3)

1 C Isotropic = 58.2638 Anisotropy = 144.5375
XX= 32.1351 YX= -28.2072 ZX= -37.6129
XY= -25.7007 YY= 65.5698 ZY= -82.4282
XZ= -35.7043 YZ= -82.4723 ZZ= 77.0865
Eigenvalues: -39.4119 59.5812 154.6221
2 C Isotropic = 47.2164 Anisotropy = 113.1146
XX= 24.9925 YX= 42.5850 ZX= 28.3088
XY= 39.3949 YY= 48.4097 ZY= -62.7325
XZ= 25.5666 YZ= -63.3527 ZZ= 68.2469
Eigenvalues: -41.3217 60.3447 122.6261
3 C Isotropic = 70.1438 Anisotropy = 125.2786
XX= -7.5682 YX= 13.1224 ZX= -3.8531
XY= 9.1738 YY= 104.7345 ZY= -43.4832
XZ= -8.9990 YZ= -43.5629 ZZ= 113.2649
Eigenvalues: -8.7076 65.4760 153.6628
4 C Isotropic = 46.7912 Anisotropy = 143.6390
XX= 13.7285 YX= -13.3051 ZX= -24.3543
XY= -13.4147 YY= 60.3658 ZY= -77.0807
XZ= -24.8930 YZ= -80.1103 ZZ= 66.2794
Eigenvalues: -31.3088 29.1320 142.5506
5 C Isotropic = 57.4208 Anisotropy = 169.2909
XX= -1.3658 YX= 17.8241 ZX= 1.0230
XY= 15.6405 YY= 79.4243 ZY= -82.6409
XZ= -2.8601 YZ= -81.9545 ZZ= 94.2039
Eigenvalues: -11.1377 13.1187 170.2814
6 C Isotropic = 60.1775 Anisotropy = 174.0531
XX= -33.0245 YX= -2.8277 ZX= -23.6904
XY= -2.7718 YY= 99.1527 ZY= -68.9549
XZ= -22.8001 YZ= -66.7487 ZZ= 114.4044
Eigenvalues: -38.1764 42.4960 176.2129
7 N Isotropic = 116.6669 Anisotropy = 86.3303
XX= 63.0030 YX= -13.7513 ZX= -22.8890
XY= -16.8138 YY= 147.0768 ZY= -27.7857
XZ= -32.2115 YZ= -32.2479 ZZ= 139.9209
Eigenvalues: 48.1165 127.6637 174.2204
8 C Isotropic = 59.2065 Anisotropy = 115.8315
XX= 48.0078 YX= 27.2962 ZX= 18.7391
XY= 22.7159 YY= 58.7753 ZY= -71.1031
XZ= 12.6158 YZ= -70.9295 ZZ= 70.8365
Eigenvalues: -19.0589 60.2510 136.4275
9 C Isotropic = 75.4965 Anisotropy = 112.5762
XX= 33.5611 YX= 25.6303 ZX= 14.1664
XY= 30.1162 YY= 90.4994 ZY= -53.5568
XZ= 18.0197 YZ= -53.1394 ZZ= 102.4291
Eigenvalues: 6.1597 69.7826 150.5473
10 C Isotropic = 66.1991 Anisotropy = 94.8158
XX= -0.4693 YX= -10.8936 ZX= 32.9656
XY= -9.2009 YY= 81.3659 ZY= 16.9987
XZ= 33.4391 YZ= 12.8162 ZZ= 117.7006
Eigenvalues: -11.1495 80.3372 129.4096
11 Br Isotropic = 1894.8170 Anisotropy = 1574.6538
XX= 1870.3871 YX= -550.2447 ZX= -440.2728
XY= -534.4053 YY= 2018.3597 ZY= 574.3783
XZ= -434.1842 YZ= 575.9334 ZZ= 1795.7041
Eigenvalues: 1320.7454 1419.1194 2944.5862
12 C Isotropic = 26.8155 Anisotropy = 144.4269
XX= 21.5136 YX= -2.0868 ZX= 23.8697

XY= -28.4151 YY= -38.8528 ZY= 59.5053
XZ= 31.1455 YZ= 55.5718 ZZ= 97.7858
Eigenvalues: -66.4434 23.7899 123.1001
13 N Isotropic = -143.6091 Anisotropy = 255.4124
XX= -147.0831 YX= 47.8568 ZX= 26.0261
XY= 39.0890 YY= -276.3614 ZY= 90.0335
XZ= 25.5262 YZ= 85.0059 ZZ= -7.3830
Eigenvalues: -309.7727 -147.7205 26.6658
14 O Isotropic = -61.7232 Anisotropy = 245.7515
XX= -129.2113 YX= 47.5815 ZX= 39.8337
XY= 56.6340 YY= -118.8573 ZY= 61.9283
XZ= 53.5612 YZ= 74.9194 ZZ= 62.8990
Eigenvalues: -177.1254 -110.1554 102.1111
15 C Isotropic = 29.0420 Anisotropy = 69.1230
XX= 26.1414 YX= -54.5768 ZX= 30.8945
XY= -45.6065 YY= 17.6316 ZY= 28.1343
XZ= 10.9539 YZ= 38.5852 ZZ= 43.3530
Eigenvalues: -45.3693 57.3713 75.1240
16 I Isotropic = 3658.4948 Anisotropy = 2193.9828
XX= 3023.2974 YX= 797.4819 ZX= -274.3551
XY= 905.0412 YY= 4376.1494 ZY= -636.4187
XZ= -242.1705 YZ= -709.2209 ZZ= 3576.0375
Eigenvalues: 2607.5367 3246.7977 5121.1500
17 C Isotropic = 62.9824 Anisotropy = 104.0587
XX= 39.0536 YX= -24.9975 ZX= 13.9608
XY= -14.1763 YY= 31.4422 ZY= 35.9127
XZ= 10.0296 YZ= 38.3069 ZZ= 118.4514
Eigenvalues: 3.4494 53.1429 132.3549
18 N Isotropic = 98.2536 Anisotropy = 127.5634
XX= 19.3352 YX= 32.6615 ZX= -2.2854
XY= 27.8751 YY= 99.1700 ZY= 28.1989
XZ= -0.9236 YZ= 19.3696 ZZ= 176.2558
Eigenvalues: 8.6481 102.8169 183.2959
19 C Isotropic = 63.7712 Anisotropy = 119.2624
XX= 50.4346 YX= -18.9843 ZX= 12.0819
XY= -27.7522 YY= 14.9116 ZY= 47.3702
XZ= 10.9968 YZ= 46.6384 ZZ= 125.9675
Eigenvalues: -12.9183 60.9525 143.2795
20 C Isotropic = 72.7078 Anisotropy = 135.1312
XX= 52.2427 YX= 22.3085 ZX= -1.4817
XY= 25.8446 YY= 20.5066 ZY= 48.9688
XZ= -4.3724 YZ= 49.8125 ZZ= 145.3740
Eigenvalues: -6.2911 61.6192 162.7952
21 C Isotropic = 68.3013 Anisotropy = 147.0807
XX= -4.8642 YX= -7.5142 ZX= 12.3571
XY= -2.4688 YY= 54.9993 ZY= 38.0024
XZ= 10.9987 YZ= 31.9587 ZZ= 154.7688
Eigenvalues: -6.7525 45.3013 166.3551
22 H Isotropic = 24.3791 Anisotropy = 9.8295
XX= 29.1167 YX= -2.3902 ZX= -1.3043
XY= -2.9546 YY= 22.1632 ZY= 3.2336
XZ= -2.2854 YZ= 3.3645 ZZ= 21.8573
Eigenvalues: 18.6742 23.5310 30.9321
23 H Isotropic = 24.1197 Anisotropy = 9.7973
XX= 23.8631 YX= -0.5705 ZX= 0.0117
XY= -0.2418 YY= 25.0977 ZY= 6.4067
XZ= 0.1483 YZ= 6.2674 ZZ= 23.3984
Eigenvalues: 17.8365 23.8714 30.6513

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 24  H    Isotropic =    24.3264   Anisotropy =     9.5355
XX=    23.0383   YX=    -0.9661   ZX=    -1.1016
XY=    -1.4651   YY=    24.4535   ZY=     5.2981
XZ=    -2.7841   YZ=     4.7397   ZZ=    25.4873
Eigenvalues:    19.8653    22.4304    30.6834
 25  H    Isotropic =    23.8735   Anisotropy =     9.7993
XX=    30.0580   YX=    -0.3661   ZX=     1.4356
XY=     0.3939   YY=    21.6139   ZY=     4.6182
XZ=     1.9204   YZ=     4.3873   ZZ=    19.9486
Eigenvalues:    16.0837    25.1305    30.4064
 26  H    Isotropic =    24.4427   Anisotropy =     6.4667
XX=    27.5986   YX=    -0.5318   ZX=     2.5500
XY=    -1.7822   YY=    23.3847   ZY=     0.8781
XZ=     2.7227   YZ=     1.8301   ZZ=    22.3450
Eigenvalues:    20.3066    24.2678    28.7539
 27  H    Isotropic =    22.8836   Anisotropy =     7.6610
XX=    27.5415   YX=    -1.2590   ZX=    -0.7855
XY=    -1.1367   YY=    24.7102   ZY=    -3.0288
XZ=    -0.6033   YZ=    -2.6009   ZZ=    16.3990
Eigenvalues:    15.4496    25.2102    27.9909
 28  H    Isotropic =    24.8043   Anisotropy =     3.8322
XX=    26.2135   YX=     0.9937   ZX=    -0.8870
XY=     0.0891   YY=    25.9297   ZY=    -1.7252
XZ=    -1.0384   YZ=    -1.8474   ZZ=    22.2697
Eigenvalues:    21.4403    25.6135    27.3591
 29  H    Isotropic =    25.5666   Anisotropy =     4.2466
XX=    26.2688   YX=     0.6937   ZX=    -0.8633
XY=     0.7278   YY=    26.5369   ZY=    -2.0272
XZ=    -1.4849   YZ=    -2.1929   ZZ=    23.8941
Eigenvalues:    22.5888    25.7133    28.3977
 30  H    Isotropic =    25.7875   Anisotropy =    11.6860
XX=    24.1071   YX=     0.2960   ZX=    -1.8231
XY=     3.7098   YY=    27.9012   ZY=    -5.8897
XZ=    -5.2980   YZ=    -4.6330   ZZ=    25.3543
Eigenvalues:    20.2830    23.5014    33.5782
```

Isomer 8 (conformer 4)

1 C Isotropic = 57.5888 Anisotropy = 146.1356
XX= 27.1719 YX= -31.4916 ZX= -37.5051
XY= -29.4161 YY= 58.8607 ZY= -80.3427
XZ= -35.9353 YZ= -80.4303 ZZ= 86.7339
Eigenvalues: -41.1968 58.9507 155.0126
2 C Isotropic = 46.5297 Anisotropy = 114.7305
XX= 27.1514 YX= 42.1824 ZX= 25.7607
XY= 38.8839 YY= 40.3559 ZY= -64.0039
XZ= 22.6822 YZ= -64.8557 ZZ= 72.0817
Eigenvalues: -41.9771 58.5494 123.0167
3 C Isotropic = 70.4629 Anisotropy = 124.7852
XX= -6.8339 YX= 15.0636 ZX= -1.8277
XY= 10.3203 YY= 100.4173 ZY= -42.8976
XZ= -6.1988 YZ= -42.8888 ZZ= 117.8053
Eigenvalues: -8.3243 66.0599 153.6530
4 C Isotropic = 46.8691 Anisotropy = 143.2165
XX= 11.9302 YX= -15.4413 ZX= -24.0651
XY= -15.2761 YY= 54.0743 ZY= -74.9404
XZ= -25.3918 YZ= -78.5591 ZZ= 74.6028
Eigenvalues: -31.2312 29.4918 142.3468
5 C Isotropic = 57.8132 Anisotropy = 167.9364
XX= 1.1769 YX= 18.5235 ZX= 0.0858
XY= 17.7648 YY= 70.8851 ZY= -80.5762
XZ= -4.5098 YZ= -81.7574 ZZ= 101.3775
Eigenvalues: -10.7938 14.4625 169.7708
6 C Isotropic = 60.6816 Anisotropy = 175.1609
XX= -33.6864 YX= -2.2461 ZX= -21.2597
XY= -1.5846 YY= 93.0635 ZY= -67.1718
XZ= -21.0611 YZ= -66.5352 ZZ= 122.6678
Eigenvalues: -37.6029 42.1923 177.4555
7 N Isotropic = 116.0056 Anisotropy = 86.9245
XX= 59.9026 YX= -12.9241 ZX= -20.9328
XY= -16.5534 YY= 145.4910 ZY= -26.4212
XZ= -31.0167 YZ= -32.2556 ZZ= 142.6231
Eigenvalues: 47.0713 126.9901 173.9552
8 C Isotropic = 59.3259 Anisotropy = 116.2854
XX= 50.4570 YX= 25.1327 ZX= 15.1452
XY= 21.7206 YY= 51.3755 ZY= -71.6247
XZ= 9.8466 YZ= -71.6807 ZZ= 76.1453
Eigenvalues: -18.7297 59.8580 136.8495
9 C Isotropic = 76.5242 Anisotropy = 111.6370
XX= 38.5483 YX= 26.1759 ZX= 12.4544
XY= 30.8489 YY= 84.1825 ZY= -53.3823
XZ= 15.5074 YZ= -54.1562 ZZ= 106.8418
Eigenvalues: 8.4044 70.2194 150.9488
10 C Isotropic = 66.5904 Anisotropy = 96.0774
XX= -0.5967 YX= -8.9687 ZX= 31.0254
XY= -5.9303 YY= 80.0963 ZY= 13.0047
XZ= 38.5436 YZ= 6.1333 ZZ= 120.2717
Eigenvalues: -10.9235 80.0528 130.6420
11 Br Isotropic = 1883.0725 Anisotropy = 1580.1787
XX= 1805.0034 YX= -548.5168 ZX= -406.2013
XY= -531.6108 YY= 2083.4544 ZY= 587.4494
XZ= -404.0116 YZ= 592.4926 ZZ= 1760.7596
Eigenvalues: 1310.2111 1402.4814 2936.5249
12 C Isotropic = 25.9400 Anisotropy = 143.0097
XX= 19.4458 YX= -7.0698 ZX= 23.1093

XY= -33.8567 YY= -46.4908 ZY= 46.2871
XZ= 29.3475 YZ= 43.7735 ZZ= 104.8650
Eigenvalues: -67.2922 23.8324 121.2798
13 N Isotropic = -158.6025 Anisotropy = 274.3877
XX= -153.9563 YX= 41.0110 ZX= 33.2288
XY= 30.3654 YY= -323.9867 ZY= 80.1654
XZ= 22.8148 YZ= 64.3957 ZZ= 2.1354
Eigenvalues: -343.8320 -156.2982 24.3226
14 O Isotropic = -72.2213 Anisotropy = 259.2661
XX= -142.3749 YX= 47.7516 ZX= 46.8137
XY= 59.9825 YY= -138.4684 ZY= 48.6767
XZ= 72.7913 YZ= 65.3090 ZZ= 64.1793
Eigenvalues: -194.3861 -122.9005 100.6228
15 C Isotropic = 30.6827 Anisotropy = 70.0382
XX= 26.5724 YX= -55.6296 ZX= 27.8821
XY= -45.7403 YY= 16.5562 ZY= 26.0719
XZ= 6.2811 YZ= 38.5291 ZZ= 48.9195
Eigenvalues: -43.0961 57.7694 77.3749
16 I Isotropic = 3667.5495 Anisotropy = 2187.3228
XX= 3068.6871 YX= 846.6912 ZX= -264.9002
XY= 950.8796 YY= 4388.0614 ZY= -570.0274
XZ= -191.3187 YZ= -695.3324 ZZ= 3545.9000
Eigenvalues: 2604.3380 3272.5457 5125.7647
17 C Isotropic = 62.8768 Anisotropy = 104.6108
XX= 51.0529 YX= 24.1973 ZX= -31.0398
XY= 22.1687 YY= 21.2720 ZY= 30.5473
XZ= -30.8053 YZ= 30.8794 ZZ= 116.3055
Eigenvalues: -5.9325 61.9456 132.6173
18 N Isotropic = 92.7324 Anisotropy = 139.2956
XX= 19.3613 YX= -33.8339 ZX= -41.6965
XY= -19.4967 YY= 86.1137 ZY= 12.7335
XZ= -39.0162 YZ= 8.5494 ZZ= 172.7222
Eigenvalues: 2.7355 89.8655 185.5961
19 C Isotropic = 63.7629 Anisotropy = 120.1221
XX= 60.4110 YX= 12.0226 ZX= -27.8750
XY= 23.3818 YY= 4.6292 ZY= 36.6348
XZ= -32.3862 YZ= 36.4688 ZZ= 126.2484
Eigenvalues: -14.4055 61.8499 143.8443
20 C Isotropic = 71.9479 Anisotropy = 138.5471
XX= 56.8718 YX= -28.9287 ZX= -26.3166
XY= -32.0098 YY= 9.0717 ZY= 23.7145
XZ= -31.9301 YZ= 21.5916 ZZ= 149.9002
Eigenvalues: -6.1704 57.7015 164.3126
21 C Isotropic = 70.9287 Anisotropy = 139.1627
XX= 16.3948 YX= 9.9619 ZX= -49.2273
XY= 5.0566 YY= 52.9655 ZY= 25.5344
XZ= -52.6021 YZ= 14.0538 ZZ= 143.4257
Eigenvalues: -4.8068 53.8890 163.7038
22 H Isotropic = 24.4731 Anisotropy = 10.1649
XX= 29.0458 YX= -2.5694 ZX= -1.7345
XY= -3.0348 YY= 22.4235 ZY= 3.3344
XZ= -2.5561 YZ= 3.5323 ZZ= 21.9499
Eigenvalues: 18.7313 23.4382 31.2497
23 H Isotropic = 24.1499 Anisotropy = 9.8077
XX= 23.9825 YX= -0.2547 ZX= 0.1910
XY= 0.0251 YY= 25.6648 ZY= 6.3719
XZ= 0.2129 YZ= 6.2159 ZZ= 22.8024
Eigenvalues: 17.7706 23.9907 30.6884

24 H Isotropic = 24.5547 Anisotropy = 9.2517
XX= 23.2856 YX= -0.1940 ZX= -1.9257
XY= -0.8725 YY= 24.2477 ZY= 5.2098
XZ= -3.1826 YZ= 4.2031 ZZ= 26.1310
Eigenvalues: 19.8827 23.0590 30.7226
25 H Isotropic = 23.8333 Anisotropy = 9.7738
XX= 30.1242 YX= -0.3564 ZX= 1.3188
XY= 0.3197 YY= 22.0751 ZY= 4.5865
XZ= 1.4985 YZ= 4.2342 ZZ= 19.3008
Eigenvalues: 15.9713 25.1796 30.3492
26 H Isotropic = 24.3129 Anisotropy = 6.8141
XX= 27.6420 YX= -0.8151 ZX= 2.5846
XY= -2.2976 YY= 23.7094 ZY= 0.7385
XZ= 2.6856 YZ= 1.6054 ZZ= 21.5872
Eigenvalues: 19.8734 24.2096 28.8556
27 H Isotropic = 24.2249 Anisotropy = 10.6966
XX= 25.8501 YX= 2.4941 ZX= 0.5555
XY= 5.6834 YY= 25.6242 ZY= -5.2376
XZ= -2.2252 YZ= -3.9209 ZZ= 21.2003
Eigenvalues: 17.9912 23.3275 31.3559
28 H Isotropic = 25.2347 Anisotropy = 4.7235
XX= 25.5096 YX= -0.0198 ZX= 0.5372
XY= 1.9172 YY= 26.9448 ZY= -2.0939
XZ= -0.8785 YZ= -2.5969 ZZ= 23.2498
Eigenvalues: 22.0909 25.2296 28.3837
29 H Isotropic = 25.2622 Anisotropy = 3.0735
XX= 26.3597 YX= 0.3614 ZX= 0.5140
XY= 1.1934 YY= 26.3440 ZY= -0.9246
XZ= -0.4402 YZ= -1.5047 ZZ= 23.0827
Eigenvalues: 22.6582 25.8172 27.3111
30 H Isotropic = 24.4992 Anisotropy = 4.2430
XX= 25.5610 YX= 1.0998 ZX= -0.0133
XY= 1.0539 YY= 26.6716 ZY= -0.9621
XZ= 0.8131 YZ= 0.4591 ZZ= 21.2650
Eigenvalues: 21.2047 24.9650 27.3279

Isomer 9 (conformer 1)

1 C Isotropic = 56.2328 Anisotropy = 146.4218
XX= -11.7839 YX= 40.6280 ZX= -18.3827
XY= 43.2568 YY= 58.8057 ZY= 54.9986
XZ= -19.8632 YZ= 55.2746 ZZ= 121.6764
Eigenvalues: -42.3372 57.1882 153.8473
2 C Isotropic = 46.2740 Anisotropy = 115.5920
XX= -9.7964 YX= -36.6055 ZX= 26.8090
XY= -40.2880 YY= 52.2092 ZY= 43.8771
XZ= 27.9325 YZ= 43.4419 ZZ= 96.4092
Eigenvalues: -42.5155 58.0022 123.3353
3 C Isotropic = 70.2417 Anisotropy = 125.1461
XX= 66.2254 YX= -2.6115 ZX= 4.5343
XY= -6.3655 YY= 33.5964 ZY= 71.2805
XZ= 6.8343 YZ= 71.8710 ZZ= 110.9033
Eigenvalues: -9.6996 66.7522 153.6724
4 C Isotropic = 47.1397 Anisotropy = 139.0340
XX= -11.4440 YX= 26.2504 ZX= -10.9434
XY= 27.6151 YY= 46.1499 ZY= 54.9695
XZ= -11.4801 YZ= 56.1601 ZZ= 106.7134
Eigenvalues: -30.6066 32.1967 139.8291
5 C Isotropic = 59.7042 Anisotropy = 162.3075
XX= 5.0857 YX= -11.9126 ZX= 12.6945
XY= -12.8697 YY= 48.5284 ZY= 71.5108
XZ= 13.3877 YZ= 70.4643 ZZ= 125.4986
Eigenvalues: -11.7215 22.9250 167.9092
6 C Isotropic = 58.7352 Anisotropy = 172.2127
XX= 36.2021 YX= 13.0206 ZX= -2.8115
XY= 18.0539 YY= 20.2582 ZY= 90.3762
XZ= -3.7746 YZ= 90.8127 ZZ= 119.7452
Eigenvalues: -36.4723 39.1342 173.5437
7 N Isotropic = 111.7867 Anisotropy = 89.1924
XX= 112.5013 YX= 29.3311 ZX= -15.9015
XY= 22.7697 YY= 81.0938 ZY= 53.1100
XZ= -11.9911 YZ= 49.9720 ZZ= 141.7651
Eigenvalues: 39.6476 124.4643 171.2484
8 C Isotropic = 59.9495 Anisotropy = 119.7253
XX= -1.7567 YX= -9.3244 ZX= 9.7310
XY= -19.7214 YY= 63.9027 ZY= 45.4458
XZ= 13.3617 YZ= 36.1933 ZZ= 117.7024
Eigenvalues: -8.4503 48.5324 139.7664
9 C Isotropic = 75.8922 Anisotropy = 109.3284
XX= 34.7548 YX= -21.5447 ZX= 16.3697
XY= -12.7369 YY= 71.0421 ZY= 45.9303
XZ= 12.1727 YZ= 45.2487 ZZ= 121.8796
Eigenvalues: 16.9336 61.9652 148.7778
10 C Isotropic = 16.7199 Anisotropy = 123.6923
XX= 1.8364 YX= 23.2963 ZX= -1.5630
XY= 0.4931 YY= -17.9408 ZY= 61.2857
XZ= 6.2683 YZ= 61.4426 ZZ= 66.2641
Eigenvalues: -51.9227 2.9010 99.1814
11 Br Isotropic = 1888.1042 Anisotropy = 1579.2272
XX= 2527.8804 YX= 553.8843 ZX= -376.8765
XY= 571.3283 YY= 1670.2774 ZY= -234.4547
XZ= -386.1901 YZ= -230.8465 ZZ= 1466.1547
Eigenvalues: 1313.7153 1409.6750 2940.9223
12 C Isotropic = 73.5078 Anisotropy = 77.8018
XX= 48.8282 YX= 20.7303 ZX= -2.7744

XY= 27.9511 YY= 59.0907 ZY= 29.4023
XZ= -11.8637 YZ= 28.4205 ZZ= 112.6046
Eigenvalues: 22.3360 72.8118 125.3757
 13 C Isotropic = 26.9466 Anisotropy = 78.7385
XX= 28.4609 YX= -61.6816 ZX= 39.9192
XY= -36.4203 YY= 3.4804 ZY= 42.9851
XZ= 23.3404 YZ= 53.3202 ZZ= 48.8985
Eigenvalues: -63.9212 65.3221 79.4389
 14 N Isotropic = -134.2929 Anisotropy = 263.0702
XX= -206.6386 YX= -80.8301 ZX= 64.4302
XY= -61.1998 YY= -168.2531 ZY= 113.9138
XZ= 70.1971 YZ= 120.6099 ZZ= -27.9871
Eigenvalues: -317.3769 -126.5890 41.0872
 15 O Isotropic = -75.4812 Anisotropy = 276.4485
XX= -166.3353 YX= 58.6587 ZX= -2.7775
XY= 55.1969 YY= -109.4165 ZY= 109.0826
XZ= 4.6025 YZ= 112.2200 ZZ= 49.3081
Eigenvalues: -217.6301 -117.6314 108.8178
 16 I Isotropic = 3754.2728 Anisotropy = 2055.0843
XX= 3805.8843 YX= 950.4177 ZX= -597.1998
XY= 1022.7944 YY= 3833.3029 ZY= -354.2304
XZ= -603.4476 YZ= -394.6204 ZZ= 3623.6311
Eigenvalues: 2787.8690 3350.6203 5124.3290
 17 C Isotropic = 63.8499 Anisotropy = 107.7931
XX= 50.0743 YX= 45.2948 ZX= -14.7327
XY= 49.9124 YY= 39.3827 ZY= -39.4932
XZ= -14.6873 YZ= -37.3704 ZZ= 102.0927
Eigenvalues: -6.8925 62.7302 135.7120
 18 N Isotropic = 93.5502 Anisotropy = 115.9502
XX= 77.8202 YX= -10.4270 ZX= -52.6903
XY= -21.3259 YY= 94.9892 ZY= -57.0306
XZ= -60.3816 YZ= -53.8280 ZZ= 107.8413
Eigenvalues: 7.2959 102.5044 170.8504
 19 C Isotropic = 66.6589 Anisotropy = 116.4603
XX= 44.5811 YX= 59.6083 ZX= -16.3909
XY= 48.4020 YY= 46.6609 ZY= -36.6782
XZ= -22.0092 YZ= -35.8937 ZZ= 108.7348
Eigenvalues: -9.7076 65.3853 144.2991
 20 C Isotropic = 70.9176 Anisotropy = 139.2726
XX= 22.3312 YX= 31.5923 ZX= -56.0966
XY= 35.3470 YY= 82.4266 ZY= -33.6911
XZ= -56.6473 YZ= -38.5238 ZZ= 107.9949
Eigenvalues: -8.2183 57.2050 163.7660
 21 C Isotropic = 69.6193 Anisotropy = 139.1105
XX= 71.7273 YX= 20.2760 ZX= -34.9758
XY= 22.7857 YY= 38.2394 ZY= -69.0223
XZ= -32.6710 YZ= -70.4825 ZZ= 98.8912
Eigenvalues: -7.4985 53.9968 162.3596
 22 H Isotropic = 24.0434 Anisotropy = 9.9954
XX= 24.8135 YX= 2.6006 ZX= -1.7739
XY= 2.4134 YY= 26.2378 ZY= -4.8353
XZ= -1.6673 YZ= -4.8459 ZZ= 21.0788
Eigenvalues: 18.1675 23.2557 30.7070
 23 H Isotropic = 24.2014 Anisotropy = 10.3892
XX= 31.1100 YX= -0.6528 ZX= -0.0846
XY= 0.0244 YY= 22.2143 ZY= -2.6488
XZ= -0.6394 YZ= -2.6520 ZZ= 19.2801
Eigenvalues: 17.7013 23.7755 31.1276

24 H Isotropic = 23.0040 Anisotropy = 10.2523
XX= 29.1097 YX= 1.3262 ZX= -1.1753
XY= 1.9472 YY= 21.9588 ZY= -3.2735
XZ= -1.5699 YZ= -3.0800 ZZ= 17.9435
Eigenvalues: 16.1794 22.9938 29.8388
25 H Isotropic = 24.0470 Anisotropy = 8.8466
XX= 26.5739 YX= -0.7540 ZX= 0.0384
XY= 0.0112 YY= 25.9933 ZY= -6.2045
XZ= -0.6328 YZ= -6.5816 ZZ= 19.5739
Eigenvalues: 15.6117 26.5846 29.9448
26 H Isotropic = 24.8767 Anisotropy = 12.5628
XX= 27.3708 YX= 2.9641 ZX= -2.7486
XY= 2.7009 YY= 25.6392 ZY= -5.2472
XZ= -5.2958 YZ= -5.7769 ZZ= 21.6201
Eigenvalues: 17.4211 23.9572 33.2519
27 H Isotropic = 24.0938 Anisotropy = 4.3946
XX= 25.2145 YX= -0.3868 ZX= 2.0609
XY= -1.3826 YY= 24.7080 ZY= 2.9232
XZ= 0.4310 YZ= 3.6497 ZZ= 22.3589
Eigenvalues: 19.6256 25.6322 27.0235
28 H Isotropic = 24.6898 Anisotropy = 3.9279
XX= 25.7914 YX= -0.8259 ZX= 1.2371
XY= -2.2932 YY= 25.6000 ZY= 1.0212
XZ= -0.1871 YZ= 1.4256 ZZ= 22.6779
Eigenvalues: 21.9291 24.8318 27.3084
29 H Isotropic = 25.0181 Anisotropy = 2.8266
XX= 26.1930 YX= -0.7246 ZX= 1.3919
XY= -0.9454 YY= 25.4581 ZY= 0.5548
XZ= 0.9948 YZ= 0.5944 ZZ= 23.4031
Eigenvalues: 22.7050 25.4468 26.9025
30 H Isotropic = 25.1098 Anisotropy = 5.9823
XX= 26.0528 YX= -1.1419 ZX= 2.3445
XY= -0.2776 YY= 24.5935 ZY= -1.3463
XZ= 4.2058 YZ= -1.0626 ZZ= 24.6832
Eigenvalues: 21.9238 24.3076 29.0980

Isomer 9 (conformer 2)

1 C Isotropic = 56.6790 Anisotropy = 145.1158
XX= -10.3442 YX= 18.0055 ZX= -52.8272
XY= 18.6348 YY= 71.9876 ZY= 52.9737
XZ= -52.0153 YZ= 53.4672 ZZ= 108.3935
Eigenvalues: -42.6530 59.2670 153.4228
2 C Isotropic = 46.6118 Anisotropy = 114.8641
XX= 4.1674 YX= -53.0510 ZX= -1.0432
XY= -57.8176 YY= 33.3008 ZY= 35.8559
XZ= 0.9573 YZ= 37.1504 ZZ= 102.3673
Eigenvalues: -42.1858 58.8333 123.1879
3 C Isotropic = 70.6760 Anisotropy = 124.3303
XX= 70.7850 YX= -7.3525 ZX= -16.7557
XY= -11.5147 YY= 27.8594 ZY= 67.4447
XZ= -13.8849 YZ= 65.5055 ZZ= 113.3835
Eigenvalues: -8.4313 66.8964 153.5629
4 C Isotropic = 46.5530 Anisotropy = 138.5142
XX= -9.5006 YX= 6.8056 ZX= -39.5329
XY= 4.9229 YY= 48.3269 ZY= 51.2520
XZ= -42.5963 YZ= 50.2169 ZZ= 100.8328
Eigenvalues: -30.3593 31.1226 138.8958
5 C Isotropic = 60.4426 Anisotropy = 161.9106
XX= 14.8823 YX= -32.4513 ZX= -21.1334
XY= -32.9761 YY= 41.6736 ZY= 64.5668
XZ= -19.7185 YZ= 66.6759 ZZ= 124.7720
Eigenvalues: -11.9223 24.8671 168.3830
6 C Isotropic = 58.6882 Anisotropy = 176.1455
XX= 34.9980 YX= -0.1750 ZX= -34.8913
XY= 2.5906 YY= 28.7042 ZY= 89.4275
XZ= -37.7786 YZ= 90.2910 ZZ= 112.3625
Eigenvalues: -35.0206 34.9667 176.1185
7 N Isotropic = 111.9775 Anisotropy = 91.8218
XX= 110.0203 YX= 25.3482 ZX= -30.0077
XY= 12.6140 YY= 92.6953 ZY= 48.1092
XZ= -31.3841 YZ= 56.9234 ZZ= 133.2170
Eigenvalues: 40.5849 122.1555 173.1921
8 C Isotropic = 59.0782 Anisotropy = 119.1314
XX= 1.9603 YX= -32.0472 ZX= -16.0157
XY= -40.4632 YY= 62.2180 ZY= 33.5208
XZ= -10.3580 YZ= 39.7504 ZZ= 113.0562
Eigenvalues: -15.1679 53.9033 138.4991
9 C Isotropic = 75.9109 Anisotropy = 106.1533
XX= 40.7112 YX= -36.0440 ZX= -3.1243
XY= -32.0001 YY= 64.2998 ZY= 38.7815
XZ= -5.0891 YZ= 41.0582 ZZ= 122.7217
Eigenvalues: 12.3426 68.7102 146.6797
10 C Isotropic = 19.1595 Anisotropy = 122.8204
XX= -20.0560 YX= -25.0598 ZX= 40.8387
XY= -4.4475 YY= -0.0793 ZY= 38.1016
XZ= 27.7690 YZ= 44.0555 ZZ= 77.6138
Eigenvalues: -48.5394 4.9780 101.0398
11 Br Isotropic = 1889.3067 Anisotropy = 1574.7978
XX= 2361.1199 YX= 729.3464 ZX= -134.4059
XY= 738.4644 YY= 1936.3994 ZY= -152.4870
XZ= -144.3108 YZ= -153.9104 ZZ= 1370.4008
Eigenvalues: 1320.9067 1407.8415 2939.1719
12 C Isotropic = 70.9524 Anisotropy = 85.8500
XX= 25.0232 YX= 11.4690 ZX= 25.1557

XY= 1.5032 YY= 76.8876 ZY= 19.8457
XZ= 30.7326 YZ= 21.0074 ZZ= 110.9465
Eigenvalues: 16.7317 67.9398 128.1858
 13 C Isotropic = 27.6315 Anisotropy = 77.2286
XX= 63.1299 YX= -5.5481 ZX= 7.4224
XY= -36.9805 YY= -44.7020 ZY= 49.2141
XZ= 8.9158 YZ= 35.7902 ZZ= 64.4667
Eigenvalues: -63.3938 67.1711 79.1173
 14 N Isotropic = -137.7928 Anisotropy = 275.1310
XX= -114.3224 YX= 14.3224 ZX= 29.7895
XY= 18.4412 YY= -295.3218 ZY= 119.1551
XZ= 59.1969 YZ= 95.7682 ZZ= -3.7344
Eigenvalues: -330.6596 -128.3468 45.6278
 15 O Isotropic = -76.3975 Anisotropy = 257.3603
XX= -195.5414 YX= 25.6419 ZX= 57.0033
XY= 30.9654 YY= -87.4934 ZY= 53.5208
XZ= 71.5217 YZ= 73.6920 ZZ= 53.8423
Eigenvalues: -212.5711 -111.7975 95.1760
 16 I Isotropic = 3738.2682 Anisotropy = 2042.1340
XX= 2802.1124 YX= 92.3635 ZX= 46.0293
XY= 80.7644 YY= 4942.5744 ZY= -529.1923
XZ= 148.1467 YZ= -478.2971 ZZ= 3470.1176
Eigenvalues: 2774.8958 3340.2179 5099.6908
 17 C Isotropic = 63.7832 Anisotropy = 109.2389
XX= 28.2055 YX= 28.5246 ZX= 36.2307
XY= 25.5235 YY= 125.2662 ZY= 11.6848
XZ= 39.5227 YZ= 9.1199 ZZ= 37.8780
Eigenvalues: -6.5995 61.3400 136.6092
 18 N Isotropic = 87.6326 Anisotropy = 127.5823
XX= 87.2734 YX= 32.1052 ZX= -24.1820
XY= 42.4314 YY= 148.3915 ZY= 42.3052
XZ= -37.6097 YZ= 50.3496 ZZ= 27.2329
Eigenvalues: -7.1817 97.3920 172.6874
 19 C Isotropic = 65.3936 Anisotropy = 120.0984
XX= 14.9746 YX= 27.4685 ZX= 41.0241
XY= 30.1397 YY= 134.4694 ZY= 8.4267
XZ= 31.0842 YZ= 16.2062 ZZ= 46.7369
Eigenvalues: -10.7529 61.4745 145.4592
 20 C Isotropic = 71.5745 Anisotropy = 139.1457
XX= 9.8569 YX= 47.8764 ZX= -8.6314
XY= 42.9820 YY= 145.8677 ZY= 22.5166
XZ= -5.2011 YZ= 27.8893 ZZ= 58.9988
Eigenvalues: -6.9996 57.3847 164.3383
 21 C Isotropic = 69.3596 Anisotropy = 141.7011
XX= 61.3869 YX= 28.6352 ZX= 15.8102
XY= 29.3020 YY= 147.1407 ZY= 29.6931
XZ= 22.2676 YZ= 33.4410 ZZ= -0.4489
Eigenvalues: -9.4717 53.7234 163.8270
 22 H Isotropic = 24.5490 Anisotropy = 12.1331
XX= 23.6832 YX= 3.7859 ZX= -0.2409
XY= 3.8494 YY= 29.5553 ZY= -4.3746
XZ= 0.2233 YZ= -4.0540 ZZ= 20.4087
Eigenvalues: 18.3272 22.6822 32.6377
 23 H Isotropic = 24.2339 Anisotropy = 9.7061
XX= 30.1187 YX= 1.3064 ZX= 2.3639
XY= 1.6632 YY= 23.0455 ZY= -2.4333
XZ= 2.0882 YZ= -2.3491 ZZ= 19.5374
Eigenvalues: 17.7544 24.2427 30.7047

24 H Isotropic = 25.2079 Anisotropy = 13.5834
XX= 25.4970 YX= 5.1383 ZX= 1.9167
XY= 2.9474 YY= 32.3432 ZY= -0.1286
XZ= 1.9691 YZ= 0.2292 ZZ= 17.7834
Eigenvalues: 17.2626 24.0975 34.2635
25 H Isotropic = 23.8157 Anisotropy = 9.6020
XX= 25.6458 YX= -0.5937 ZX= 2.5005
XY= -0.4508 YY= 26.5678 ZY= -5.9957
XZ= 1.8224 YZ= -5.4698 ZZ= 19.2334
Eigenvalues: 15.8153 25.4147 30.2170
26 H Isotropic = 23.8866 Anisotropy = 6.0719
XX= 25.0895 YX= 0.6723 ZX= 0.4445
XY= -0.5473 YY= 25.0976 ZY= -3.7180
XZ= 1.7182 YZ= -4.6139 ZZ= 21.4727
Eigenvalues: 18.6055 25.1198 27.9346
27 H Isotropic = 24.1440 Anisotropy = 3.2104
XX= 24.0213 YX= -2.6763 ZX= 0.6686
XY= -2.6781 YY= 22.5095 ZY= -1.7974
XZ= -0.8997 YZ= 0.5665 ZZ= 25.9013
Eigenvalues: 20.4260 25.7218 26.2843
28 H Isotropic = 24.9945 Anisotropy = 3.7040
XX= 26.0321 YX= -1.6504 ZX= -0.5644
XY= -1.4087 YY= 23.9000 ZY= -1.1731
XZ= -2.3837 YZ= 0.6515 ZZ= 25.0513
Eigenvalues: 22.6893 24.8304 27.4638
29 H Isotropic = 25.0774 Anisotropy = 2.9076
XX= 26.5013 YX= -1.0567 ZX= -0.1556
XY= -1.3501 YY= 24.1874 ZY= -1.7219
XZ= -0.8049 YZ= -0.8537 ZZ= 24.5434
Eigenvalues: 22.6689 25.5475 27.0158
30 H Isotropic = 24.9229 Anisotropy = 6.7088
XX= 29.0809 YX= 0.6384 ZX= 0.7838
XY= 1.4144 YY= 22.8627 ZY= -1.3461
XZ= 1.7170 YZ= -2.3020 ZZ= 22.8252
Eigenvalues: 20.7097 24.6637 29.3954

Isomer 9 (conformer 3)

1 C Isotropic = 56.2536 Anisotropy = 146.4104
XX= -3.7190 YX= 46.9659 ZX= -7.5979
XY= 49.7006 YY= 19.4390 ZY= 9.4025
XZ= -7.9506 YZ= 9.8115 ZZ= 153.0408
Eigenvalues: -42.5838 57.4841 153.8606
2 C Isotropic = 46.4100 Anisotropy = 115.1988
XX= -17.5110 YX= -41.8509 ZX= -1.7997
XY= -45.5686 YY= 33.8402 ZY= 3.9210
XZ= -2.6528 YZ= 3.7971 ZZ= 122.9007
Eigenvalues: -42.5284 58.5492 123.2092
3 C Isotropic = 70.1722 Anisotropy = 125.0507
XX= 64.6341 YX= -11.0712 ZX= -1.9723
XY= -15.6334 YY= -7.0424 ZY= 8.8966
XZ= -2.0528 YZ= 9.4945 ZZ= 152.9249
Eigenvalues: -9.9134 66.8907 153.5393
4 C Isotropic = 47.0998 Anisotropy = 139.5277
XX= -6.7421 YX= 29.2299 ZX= -5.8803
XY= 30.8938 YY= 8.6557 ZY= 8.4613
XZ= -6.4101 YZ= 9.4911 ZZ= 139.3857
Eigenvalues: -30.7067 31.8878 140.1182
5 C Isotropic = 59.3283 Anisotropy = 162.2956
XX= 1.4975 YX= -16.7233 ZX= -4.0598
XY= -17.5748 YY= 9.5103 ZY= 8.6417
XZ= -3.5923 YZ= 7.5259 ZZ= 166.9771
Eigenvalues: -12.1301 22.5897 167.5254
6 C Isotropic = 58.5713 Anisotropy = 172.0135
XX= 37.9138 YX= 6.2211 ZX= -4.4798
XY= 11.1959 YY= -34.6416 ZY= 12.3751
XZ= -2.8693 YZ= 12.2867 ZZ= 172.4416
Eigenvalues: -36.4418 38.9087 173.2469
7 N Isotropic = 112.5020 Anisotropy = 88.5321
XX= 117.9901 YX= 26.5089 ZX= -2.9721
XY= 19.2527 YY= 48.1471 ZY= 7.4437
XZ= 0.6340 YZ= 1.2170 ZZ= 171.3687
Eigenvalues: 41.1645 124.8181 171.5234
8 C Isotropic = 60.3710 Anisotropy = 122.9838
XX= -6.6561 YX= -14.5229 ZX= -2.7834
XY= -20.2503 YY= 46.0618 ZY= 4.3190
XZ= -8.5147 YZ= -18.5008 ZZ= 141.7072
Eigenvalues: -12.2353 50.9880 142.3601
9 C Isotropic = 76.2087 Anisotropy = 107.7721
XX= 31.4047 YX= -25.4335 ZX= -2.1347
XY= -17.1546 YY= 49.4019 ZY= 4.5573
XZ= -0.1654 YZ= 4.2771 ZZ= 147.8196
Eigenvalues: 17.2691 63.3003 148.0568
10 C Isotropic = 16.7206 Anisotropy = 123.6357
XX= -0.5350 YX= 19.4946 ZX= 4.0415
XY= -5.6821 YY= -48.3806 ZY= 1.0037
XZ= -2.3246 YZ= 4.7922 ZZ= 99.0776
Eigenvalues: -49.4085 0.4260 99.1444
11 Br Isotropic = 1891.6155 Anisotropy = 1573.0982
XX= 2638.4910 YX= 598.8397 ZX= 4.6985
XY= 617.3041 YY= 1715.4182 ZY= -4.9040
XZ= -2.5382 YZ= -5.3666 ZZ= 1320.9373
Eigenvalues: 1320.6585 1413.8405 2940.3477
12 C Isotropic = 73.1812 Anisotropy = 77.9953
XX= 50.5026 YX= 19.0471 ZX= 1.2765

XY= 29.4372 YY= 44.0514 ZY= -2.2331
XZ= -2.1382 YZ= -4.8703 ZZ= 124.9895
Eigenvalues: 22.7653 71.6002 125.1780
 13 C Isotropic = 28.7196 Anisotropy = 78.5622
XX= 23.0486 YX= -78.5553 ZX= 3.3765
XY= -48.1846 YY= -16.6196 ZY= 3.8021
XZ= 0.9843 YZ= 13.0582 ZZ= 79.7297
Eigenvalues: -63.6430 68.7073 81.0943
 14 N Isotropic = -133.3263 Anisotropy = 267.9005
XX= -220.6331 YX= -102.9373 ZX= 6.3466
XY= -86.7169 YY= -223.7884 ZY= 2.3046
XZ= 22.8017 YZ= 13.6255 ZZ= 44.4427
Eigenvalues: -317.7490 -127.5038 45.2740
 15 O Isotropic = -76.9531 Anisotropy = 273.3204
XX= -161.9233 YX= 52.0790 ZX= 9.4200
XY= 47.9741 YY= -173.3937 ZY= 0.8922
XZ= 17.9289 YZ= 4.5193 ZZ= 104.4577
Eigenvalues: -218.1689 -117.9509 105.2605
 16 I Isotropic = 3779.0853 Anisotropy = 2021.4661
XX= 4030.9192 YX= 1101.9301 ZX= -70.6687
XY= 1165.2857 YY= 3945.9510 ZY= -27.7677
XZ= -67.8473 YZ= -67.4089 ZZ= 3360.3855
Eigenvalues: 2853.6548 3356.8716 5126.7293
 17 C Isotropic = 63.2407 Anisotropy = 108.7785
XX= 16.8212 YX= 37.8773 ZX= -36.4021
XY= 33.7615 YY= 103.1176 ZY= -24.7185
XZ= -41.0761 YZ= -20.2460 ZZ= 69.7833
Eigenvalues: -8.2156 62.1780 135.7597
 18 N Isotropic = 87.0818 Anisotropy = 125.3102
XX= 103.4873 YX= 20.2634 ZX= -17.9703
XY= 25.3730 YY= 106.1801 ZY= -76.7925
XZ= -12.1578 YZ= -74.9122 ZZ= 51.5778
Eigenvalues: -1.7433 92.3667 170.6219
 19 C Isotropic = 65.1412 Anisotropy = 118.8973
XX= 13.5364 YX= 40.2454 ZX= -38.5062
XY= 47.9173 YY= 106.4826 ZY= -20.7138
XZ= -31.7704 YZ= -29.7639 ZZ= 75.4046
Eigenvalues: -11.1167 62.1343 144.4061
 20 C Isotropic = 72.7146 Anisotropy = 136.5322
XX= 42.9987 YX= 61.7800 ZX= -0.6818
XY= 58.0618 YY= 98.1788 ZY= -52.7925
XZ= -5.8578 YZ= -55.4041 ZZ= 76.9663
Eigenvalues: -5.7949 60.2026 163.7361
 21 C Isotropic = 72.1562 Anisotropy = 137.6119
XX= 54.4857 YX= 25.2312 ZX= -43.5764
XY= 23.2971 YY= 115.3716 ZY= -52.9691
XZ= -60.2329 YZ= -50.4674 ZZ= 46.6113
Eigenvalues: -6.2944 58.8655 163.8975
 22 H Isotropic = 24.0444 Anisotropy = 10.0160
XX= 25.3165 YX= 3.5232 ZX= 0.0085
XY= 3.2478 YY= 28.5872 ZY= -0.4446
XZ= 0.0380 YZ= -0.4231 ZZ= 18.2297
Eigenvalues: 18.2070 23.2046 30.7218
 23 H Isotropic = 24.2000 Anisotropy = 10.3039
XX= 30.9860 YX= -1.1150 ZX= 0.4659
XY= -0.3227 YY= 23.8049 ZY= -0.3146
XZ= 0.2640 YZ= -0.3744 ZZ= 17.8089
Eigenvalues: 17.7812 23.7495 31.0692

24 H Isotropic = 23.0083 Anisotropy = 10.3032
XX= 29.4281 YX= 1.3353 ZX= 0.3840
XY= 2.0337 YY= 23.4054 ZY= -0.1297
XZ= 0.4134 YZ= -0.0200 ZZ= 16.1914
Eigenvalues: 16.1772 22.9707 29.8771
25 H Isotropic = 24.0428 Anisotropy = 8.9755
XX= 26.4061 YX= -0.5741 ZX= 0.3301
XY= 0.4663 YY= 29.9475 ZY= -0.7167
XZ= -0.0891 YZ= -1.3906 ZZ= 15.7748
Eigenvalues: 15.6956 26.4063 30.0265
26 H Isotropic = 23.6184 Anisotropy = 12.4230
XX= 27.3126 YX= 4.5650 ZX= -0.8858
XY= 4.1665 YY= 27.5864 ZY= -0.1590
XZ= -2.8660 YZ= 0.6182 ZZ= 15.9560
Eigenvalues: 15.5735 23.3812 31.9003
27 H Isotropic = 23.7549 Anisotropy = 5.0148
XX= 22.7448 YX= -2.9440 ZX= 2.0638
XY= -3.1421 YY= 24.3804 ZY= 1.2219
XZ= 4.1927 YZ= 1.8557 ZZ= 24.1394
Eigenvalues: 18.3670 25.7996 27.0981
28 H Isotropic = 24.6342 Anisotropy = 3.9157
XX= 26.1153 YX= -2.1679 ZX= 0.9067
XY= -1.3636 YY= 24.1404 ZY= 1.7287
XZ= 1.8132 YZ= 0.8832 ZZ= 23.6469
Eigenvalues: 21.5211 25.1368 27.2446
29 H Isotropic = 25.0996 Anisotropy = 2.8873
XX= 26.1250 YX= -1.3022 ZX= 0.4175
XY= -1.2099 YY= 24.8439 ZY= 1.6387
XZ= 0.2218 YZ= 1.3524 ZZ= 24.3299
Eigenvalues: 22.7256 25.5487 27.0245
30 H Isotropic = 25.0389 Anisotropy = 5.1189
XX= 26.6307 YX= -1.1487 ZX= -0.9443
XY= -1.2621 YY= 24.9429 ZY= 1.4256
XZ= -2.5966 YZ= 2.1083 ZZ= 23.5431
Eigenvalues: 22.1640 24.5013 28.4515

Isomer 9 (conformer 4)

1 C Isotropic = 57.5003 Anisotropy = 143.6012
XX= -6.8828 YX= 16.0319 ZX= -53.3805
XY= 17.3186 YY= 72.9268 ZY= 52.5375
XZ= -54.9296 YZ= 53.3198 ZZ= 106.4569
Eigenvalues: -40.6506 59.9170 153.2344
2 C Isotropic = 47.0624 Anisotropy = 113.9072
XX= 4.8623 YX= -53.6695 ZX= -2.5247
XY= -58.7776 YY= 33.5725 ZY= 34.3944
XZ= -1.8356 YZ= 34.7045 ZZ= 102.7525
Eigenvalues: -41.5689 59.7556 123.0005
3 C Isotropic = 70.5313 Anisotropy = 124.6651
XX= 71.0432 YX= -8.4987 ZX= -17.4220
XY= -12.9304 YY= 27.6232 ZY= 66.9226
XZ= -14.6618 YZ= 65.8215 ZZ= 112.9275
Eigenvalues: -8.6579 66.6104 153.6414
4 C Isotropic = 46.6106 Anisotropy = 139.1928
XX= -8.7782 YX= 5.8891 ZX= -41.3351
XY= 4.5482 YY= 48.4161 ZY= 51.4310
XZ= -44.1927 YZ= 50.3743 ZZ= 100.1939
Eigenvalues: -30.7714 31.1974 139.4058
5 C Isotropic = 60.4216 Anisotropy = 163.5892
XX= 14.3852 YX= -33.2332 ZX= -23.5069
XY= -32.5379 YY= 39.9831 ZY= 65.3686
XZ= -18.8593 YZ= 65.1214 ZZ= 126.8965
Eigenvalues: -12.6721 24.4558 169.4810
6 C Isotropic = 59.3586 Anisotropy = 175.1236
XX= 37.3227 YX= -1.3749 ZX= -36.7296
XY= 3.2717 YY= 28.3323 ZY= 90.3659
XZ= -34.7227 YZ= 89.5877 ZZ= 112.4208
Eigenvalues: -34.8242 36.7924 176.1077
7 N Isotropic = 112.5235 Anisotropy = 90.9959
XX= 111.5067 YX= 25.2629 ZX= -30.7820
XY= 12.1076 YY= 92.5034 ZY= 48.3049
XZ= -31.5173 YZ= 55.2498 ZZ= 133.5605
Eigenvalues: 41.4185 122.9646 173.1875
8 C Isotropic = 59.0656 Anisotropy = 119.1856
XX= 2.5210 YX= -32.5694 ZX= -17.9979
XY= -41.2387 YY= 62.2218 ZY= 32.7938
XZ= -10.9436 YZ= 39.9992 ZZ= 112.4540
Eigenvalues: -15.1554 53.8295 138.5227
9 C Isotropic = 75.6671 Anisotropy = 107.2035
XX= 40.6650 YX= -36.8778 ZX= -3.8310
XY= -32.5015 YY= 63.3115 ZY= 39.1753
XZ= -5.9757 YZ= 40.8696 ZZ= 123.0247
Eigenvalues: 11.4961 68.3690 147.1361
10 C Isotropic = 17.3021 Anisotropy = 125.3652
XX= -19.0903 YX= -22.8998 ZX= 46.2192
XY= -3.3124 YY= -1.8410 ZY= 37.1120
XZ= 34.9924 YZ= 47.8696 ZZ= 72.8375
Eigenvalues: -52.3213 3.3487 100.8788
11 Br Isotropic = 1893.0283 Anisotropy = 1575.6630
XX= 2373.6543 YX= 731.2958 ZX= -113.2488
XY= 738.5340 YY= 1939.6820 ZY= -141.4516
XZ= -127.4722 YZ= -137.4308 ZZ= 1365.7485
Eigenvalues: 1322.4197 1413.1949 2943.4703
12 C Isotropic = 70.6924 Anisotropy = 84.6594
XX= 26.8658 YX= 13.1228 ZX= 30.1276

XY= 3.5712 YY= 77.8957 ZY= 18.1436
XZ= 34.2791 YZ= 19.3829 ZZ= 107.3156
Eigenvalues: 15.5157 69.4294 127.1320
 13 C Isotropic = 28.8456 Anisotropy = 78.4785
XX= 67.1263 YX= -3.3942 ZX= 5.4453
XY= -31.3107 YY= -46.1200 ZY= 53.2388
XZ= 9.7328 YZ= 35.3917 ZZ= 65.5307
Eigenvalues: -64.2848 69.6571 81.1646
 14 N Isotropic = -138.5593 Anisotropy = 276.7353
XX= -109.6747 YX= 21.4281 ZX= 35.2338
XY= 27.0377 YY= -296.7476 ZY= 114.9946
XZ= 72.8124 YZ= 90.4093 ZZ= -9.2556
Eigenvalues: -329.8730 -131.7358 45.9309
 15 O Isotropic = -81.2517 Anisotropy = 262.0457
XX= -191.4770 YX= 26.5241 ZX= 71.1794
XY= 33.6770 YY= -94.0508 ZY= 52.3126
XZ= 93.0586 YZ= 74.0272 ZZ= 41.7726
Eigenvalues: -218.3486 -118.8520 93.4454
 16 I Isotropic = 3778.9694 Anisotropy = 2052.1399
XX= 2898.3776 YX= -34.1690 ZX= 105.4582
XY= -70.7039 YY= 4965.8276 ZY= -564.5114
XZ= 181.9881 YZ= -523.7776 ZZ= 3472.7029
Eigenvalues: 2861.0928 3328.7526 5147.0627
 17 C Isotropic = 64.3524 Anisotropy = 109.7490
XX= 14.1308 YX= 44.3020 ZX= -11.1658
XY= 44.1847 YY= 120.6350 ZY= 13.2280
XZ= -19.2088 YZ= 15.4202 ZZ= 58.2914
Eigenvalues: -7.4683 63.0071 137.5184
 18 N Isotropic = 88.0777 Anisotropy = 126.8896
XX= 102.9747 YX= 21.7833 ZX= 12.1203
XY= 21.2473 YY= 163.5826 ZY= 13.2277
XZ= 23.0282 YZ= 16.7747 ZZ= -2.3243
Eigenvalues: -5.9637 97.5260 172.6707
 19 C Isotropic = 65.1434 Anisotropy = 119.3121
XX= 4.0645 YX= 46.6039 ZX= -16.5517
XY= 39.8403 YY= 131.0200 ZY= 6.0304
XZ= -4.4008 YZ= 11.6760 ZZ= 60.3458
Eigenvalues: -11.4762 62.2217 144.6848
 20 C Isotropic = 71.6915 Anisotropy = 140.2422
XX= 23.9535 YX= 38.6090 ZX= 34.2821
XY= 40.1482 YY= 152.5155 ZY= 2.6304
XZ= 30.5558 YZ= 7.6817 ZZ= 38.6056
Eigenvalues: -7.0768 56.9651 165.1864
 21 C Isotropic = 68.5656 Anisotropy = 142.3124
XX= 49.8558 YX= 37.6589 ZX= -19.1256
XY= 41.5274 YY= 147.1394 ZY= 25.2364
XZ= -27.2260 YZ= 29.6506 ZZ= 8.7015
Eigenvalues: -12.9416 55.1977 163.4405
 22 H Isotropic = 24.5866 Anisotropy = 12.1420
XX= 23.8152 YX= 3.8745 ZX= -0.1821
XY= 3.9328 YY= 29.5596 ZY= -4.2187
XZ= 0.2591 YZ= -4.1219 ZZ= 20.3851
Eigenvalues: 18.3081 22.7705 32.6813
 23 H Isotropic = 24.2425 Anisotropy = 9.6904
XX= 30.0502 YX= 1.3240 ZX= 2.5475
XY= 1.6653 YY= 23.0986 ZY= -2.4046
XZ= 2.2436 YZ= -2.3243 ZZ= 19.5788
Eigenvalues: 17.7481 24.2767 30.7028

24 H Isotropic = 25.3867 Anisotropy = 12.9512
XX= 25.9468 YX= 5.0025 ZX= 1.6837
XY= 2.9603 YY= 32.0295 ZY= 0.3323
XZ= 1.4437 YZ= -0.5544 ZZ= 18.1838
Eigenvalues: 17.8201 24.3192 34.0208
25 H Isotropic = 23.8337 Anisotropy = 9.6593
XX= 25.5327 YX= -0.4689 ZX= 2.5657
XY= -0.3576 YY= 26.5670 ZY= -5.9622
XZ= 1.9669 YZ= -5.6302 ZZ= 19.4013
Eigenvalues: 15.8386 25.3892 30.2732
26 H Isotropic = 23.9231 Anisotropy = 5.9310
XX= 25.0921 YX= 0.6344 ZX= 0.5226
XY= -0.5296 YY= 25.0753 ZY= -3.6071
XZ= 1.8436 YZ= -4.4793 ZZ= 21.6018
Eigenvalues: 18.7734 25.1187 27.8771
27 H Isotropic = 23.6245 Anisotropy = 5.1397
XX= 26.8663 YX= 0.7346 ZX= -0.2140
XY= 1.7100 YY= 18.8158 ZY= -1.6523
XZ= 0.7542 YZ= -2.8417 ZZ= 25.1914
Eigenvalues: 17.9295 25.8931 27.0510
28 H Isotropic = 24.5591 Anisotropy = 3.8702
XX= 26.5556 YX= -1.1430 ZX= -0.7459
XY= -1.8688 YY= 22.9506 ZY= -1.5817
XZ= 0.4590 YZ= -1.0440 ZZ= 24.1710
Eigenvalues: 21.7260 24.8120 27.1393
29 H Isotropic = 25.3177 Anisotropy = 2.8444
XX= 26.1287 YX= -1.2507 ZX= -0.8516
XY= -1.2805 YY= 24.3848 ZY= -0.6045
XZ= -1.0739 YZ= 0.5911 ZZ= 25.4396
Eigenvalues: 23.5929 25.1462 27.2139
30 H Isotropic = 25.5013 Anisotropy = 4.6268
XX= 25.1804 YX= -1.2973 ZX= -1.1151
XY= -1.1412 YY= 25.4920 ZY= 0.4631
XZ= -2.5728 YZ= 2.5364 ZZ= 25.8316
Eigenvalues: 23.6325 24.2857 28.5859

Isomer 10 (conformer 1)

1 C Isotropic = 57.7786 Anisotropy = 146.0034
XX= 18.2335 YX= 38.9359 ZX= -48.4790
XY= 42.8560 YY= 19.4199 ZY= 30.0678
XZ= -49.2143 YZ= 30.5549 ZZ= 135.6823
Eigenvalues: -40.1202 58.3417 155.1142
2 C Isotropic = 46.9195 Anisotropy = 114.1869
XX= -7.3242 YX= -41.1676 ZX= -36.6524
XY= -45.5672 YY= 37.0457 ZY= -3.9584
XZ= -38.5160 YZ= -2.7295 ZZ= 111.0369
Eigenvalues: -41.4790 59.1933 123.0441
3 C Isotropic = 69.5497 Anisotropy = 126.3223
XX= 69.2878 YX= -15.2603 ZX= -25.5801
XY= -21.3778 YY= -4.4496 ZY= 12.2562
XZ= -25.1841 YZ= 14.6270 ZZ= 143.8111
Eigenvalues: -9.1196 64.0042 153.7646
4 C Isotropic = 46.9150 Anisotropy = 143.9260
XX= 10.3122 YX= 22.7910 ZX= -46.7144
XY= 22.5994 YY= 7.0744 ZY= 23.0294
XZ= -50.2145 YZ= 24.2785 ZZ= 123.3583
Eigenvalues: -31.1235 29.0027 142.8657
5 C Isotropic = 58.4638 Anisotropy = 167.0684
XX= 19.1029 YX= -16.2154 ZX= -48.1837
XY= -18.7344 YY= 4.7632 ZY= 12.5156
XZ= -48.6442 YZ= 18.7495 ZZ= 151.5253
Eigenvalues: -8.9064 14.4550 169.8427
6 C Isotropic = 61.2860 Anisotropy = 174.0623
XX= 53.4465 YX= -0.4110 ZX= -39.3309
XY= 0.4683 YY= -33.1042 ZY= 24.5951
XZ= -33.9412 YZ= 25.4835 ZZ= 163.5155
Eigenvalues: -36.4947 43.0251 177.3275
7 N Isotropic = 115.3277 Anisotropy = 89.1285
XX= 128.2835 YX= 19.4948 ZX= -19.0575
XY= 13.2094 YY= 53.9736 ZY= 18.4190
XZ= -22.7342 YZ= 23.6156 ZZ= 163.7262
Eigenvalues: 45.1820 126.0545 174.7467
8 C Isotropic = 57.8546 Anisotropy = 119.5755
XX= 0.3783 YX= -19.0338 ZX= -45.7949
XY= -27.6535 YY= 51.3187 ZY= -1.1367
XZ= -44.3135 YZ= 3.1021 ZZ= 121.8668
Eigenvalues: -21.1392 57.1314 137.5716
9 C Isotropic = 76.2906 Anisotropy = 111.6057
XX= 43.1671 YX= -35.4145 ZX= -32.2447
XY= -29.2764 YY= 46.1713 ZY= 1.8759
XZ= -32.8006 YZ= 0.9653 ZZ= 139.5335
Eigenvalues: 8.1691 70.0084 150.6944
10 C Isotropic = 76.0403 Anisotropy = 79.9368
XX= 73.9644 YX= -34.5066 ZX= 28.7038
XY= -25.4818 YY= 44.9121 ZY= -9.0998
XZ= 27.6535 YZ= 0.0478 ZZ= 109.2443
Eigenvalues: 24.4527 74.3366 129.3315
11 Br Isotropic = 1886.6607 Anisotropy = 1592.7255
XX= 2581.6038 YX= 567.7760 ZX= 338.2341
XY= 583.3807 YY= 1685.5826 ZY= 141.8345
XZ= 335.3825 YZ= 140.8830 ZZ= 1392.7956
Eigenvalues: 1303.2019 1408.3025 2948.4777
12 C Isotropic = 21.5512 Anisotropy = 124.8803
XX= 6.6601 YX= -16.2550 ZX= 70.9524

XY= -34.1095 YY=   9.7673 ZY=   -6.1993
XZ=   66.9108 YZ= -12.2118 ZZ=   48.2260
Eigenvalues: -48.5040   8.3528 104.8047
 13 O   Isotropic = -70.5716   Anisotropy = 259.7783
XX= -65.1257 YX= -79.6226 ZX= 107.5145
XY= -76.7138 YY= -156.1600 ZY= -28.6202
XZ= 103.5270 YZ= -27.0241 ZZ=   9.5710
Eigenvalues: -206.2863 -108.0423 102.6140
 14 N   Isotropic = -134.3799   Anisotropy = 268.8979
XX= -130.0190 YX=   20.9664 ZX= 143.6933
XY=   40.5635 YY= -161.1777 ZY= -99.3669
XZ= 155.9134 YZ= -104.6378 ZZ= -111.9428
Eigenvalues: -325.5519 -122.4731   44.8854
 15 C   Isotropic =   27.5927   Anisotropy =   74.4152
XX=   21.4401 YX=   24.6853 ZX=   52.6851
XY=   41.4690 YY=   51.9594 ZY= -44.0595
XZ=   68.4175 YZ= -20.9470 ZZ=   9.3786
Eigenvalues: -63.9417   69.5171   77.2028
 16 C   Isotropic =   62.4457   Anisotropy = 101.8310
XX=   55.3889 YX= -22.2784 ZX=   58.6208
XY= -25.1852 YY=   48.7562 ZY=   7.4474
XZ=   57.7789 YZ=   5.4110 ZZ=   83.1918
Eigenvalues: -0.9775   57.9815 130.3330
 17 N   Isotropic =   94.9888   Anisotropy = 136.6154
XX= 118.2663 YX= -22.7855 ZX=   49.2510
XY= -10.7636 YY=   13.9376 ZY= -19.8019
XZ=   39.1681 YZ= -13.1611 ZZ= 152.7625
Eigenvalues: 10.5823   88.3184 186.0657
 18 C   Isotropic =   62.4926   Anisotropy = 119.7182
XX=   46.8467 YX= -20.4156 ZX=   74.9223
XY= -11.6811 YY=   59.9951 ZY=   -4.1487
XZ=   75.7979 YZ=   3.1692 ZZ=   80.6360
Eigenvalues: -15.4866   60.6596 142.3047
 19 C   Isotropic =   71.8237   Anisotropy = 137.5738
XX=   79.6649 YX=   13.7116 ZX=   71.4148
XY=   12.4144 YY=   36.4208 ZY= -32.9611
XZ=   71.3129 YZ= -30.7245 ZZ=   99.3856
Eigenvalues: -5.7486   57.6802 163.5396
 20 C   Isotropic =   70.5481   Anisotropy = 142.5882
XX=   86.8163 YX= -29.6680 ZX=   60.4736
XY= -29.5285 YY=   7.6366 ZY=   -2.9209
XZ=   57.9056 YZ=   -0.7827 ZZ= 117.1915
Eigenvalues: -5.3505   51.3879 165.6070
 21 I   Isotropic = 3789.3330   Anisotropy = 2011.4485
XX= 3737.5657 YX= -777.0882 ZX= -569.9488
XY= -685.7629 YY= 3515.0586 ZY= 749.0077
XZ= -575.6665 YZ= 608.3814 ZZ= 4115.3746
Eigenvalues: 2859.6567 3378.0436 5130.2987
 22 H   Isotropic =   24.3067   Anisotropy =   9.9596
XX=   25.3944 YX=   4.1255 ZX=   2.1962
XY=   3.2589 YY=   28.1284 ZY=   0.0860
XZ=   2.3870 YZ=   0.7885 ZZ=   19.3974
Eigenvalues: 18.5466   23.4271   30.9465
 23 H   Isotropic =   24.0893   Anisotropy =   9.8524
XX=   29.4225 YX=   -0.6343 ZX=   3.7700
XY=   -0.2514 YY=   23.9588 ZY=   -0.7871
XZ=   3.6398 YZ=   -0.7042 ZZ=   18.8865
Eigenvalues: 17.6610   23.9493   30.6576

24 H Isotropic = 24.3135 Anisotropy = 9.5540
XX= 28.4733 YX= 1.7294 ZX= 4.2480
XY= 0.6206 YY= 22.6147 ZY= 0.1430
XZ= 3.8691 YZ= 1.9399 ZZ= 21.8525
Eigenvalues: 19.8506 22.4071 30.6828
25 H Isotropic = 23.7795 Anisotropy = 9.5063
XX= 24.6133 YX= -0.2629 ZX= 2.3927
XY= 0.4981 YY= 29.8673 ZY= -1.8335
XZ= 2.0715 YZ= -1.7569 ZZ= 16.8578
Eigenvalues: 16.0359 25.1855 30.1170
26 H Isotropic = 24.3146 Anisotropy = 6.3251
XX= 24.2665 YX= 1.2423 ZX= -0.4864
XY= -0.2277 YY= 27.1406 ZY= -2.8178
XZ= 0.3650 YZ= -3.2685 ZZ= 21.5366
Eigenvalues: 20.1965 24.2159 28.5314
27 H Isotropic = 23.9872 Anisotropy = 15.1310
XX= 20.1421 YX= -1.8618 ZX= -6.4604
XY= 0.2326 YY= 27.2991 ZY= 4.3514
XZ= -4.1296 YZ= 9.2758 ZZ= 24.5204
Eigenvalues: 15.5042 22.3828 34.0746
28 H Isotropic = 25.0883 Anisotropy = 5.2817
XX= 24.1713 YX= -0.5483 ZX= -2.9348
XY= 0.6304 YY= 25.8041 ZY= 1.0102
XZ= -2.9602 YZ= 2.9540 ZZ= 25.2896
Eigenvalues: 21.3237 25.3318 28.6094
29 H Isotropic = 25.2199 Anisotropy = 2.9737
XX= 24.7648 YX= -0.0643 ZX= -1.9731
XY= 0.5300 YY= 26.3834 ZY= 0.5955
XZ= -1.8986 YZ= 1.6915 ZZ= 24.5114
Eigenvalues: 22.4417 26.0156 27.2023
30 H Isotropic = 24.3343 Anisotropy = 5.0526
XX= 24.3596 YX= -0.3903 ZX= -2.8283
XY= -0.5364 YY= 25.6148 ZY= 1.8710
XZ= -2.5840 YZ= 1.8629 ZZ= 23.0285
Eigenvalues: 20.6041 24.6961 27.7027

Isomer 10 (conformer 2)

1 C Isotropic = 58.4091 Anisotropy = 144.4095
XX= 20.4834 YX= 36.8302 ZX= -51.4550
XY= 41.0043 YY= 22.8775 ZY= 33.2268
XZ= -52.3523 YZ= 33.2285 ZZ= 131.8663
Eigenvalues: -38.8157 59.3609 154.6821
2 C Isotropic = 47.5130 Anisotropy = 112.2210
XX= -5.1221 YX= -42.7389 ZX= -37.8016
XY= -46.9559 YY= 38.4577 ZY= -3.7840
XZ= -38.9675 YZ= -2.5958 ZZ= 109.2033
Eigenvalues: -41.1390 61.3509 122.3270
3 C Isotropic = 69.6149 Anisotropy = 126.0623
XX= 71.1333 YX= -16.2703 ZX= -26.4339
XY= -21.8326 YY= -4.1886 ZY= 15.2775
XZ= -26.0024 YZ= 18.4794 ZZ= 141.8999
Eigenvalues: -9.4894 64.6775 153.6564
4 C Isotropic = 46.8398 Anisotropy = 143.9281
XX= 11.7057 YX= 21.0724 ZX= -49.5935
XY= 21.0016 YY= 8.4486 ZY= 26.1481
XZ= -52.5933 YZ= 26.5273 ZZ= 120.3652
Eigenvalues: -31.1163 28.8439 142.7918
5 C Isotropic = 58.5885 Anisotropy = 167.6229
XX= 19.9626 YX= -17.5112 ZX= -50.9666
XY= -21.2293 YY= 5.4852 ZY= 15.5086
XZ= -49.3205 YZ= 17.8565 ZZ= 150.3178
Eigenvalues: -10.1379 15.5663 170.3371
6 C Isotropic = 60.7606 Anisotropy = 173.4690
XX= 54.5729 YX= -1.4840 ZX= -41.6197
XY= -1.3810 YY= -31.9452 ZY= 29.8959
XZ= -36.2897 YZ= 29.0310 ZZ= 159.6540
Eigenvalues: -36.6021 42.4773 176.4066
7 N Isotropic = 116.2626 Anisotropy = 87.1235
XX= 129.9576 YX= 18.5617 ZX= -19.5955
XY= 12.3296 YY= 56.5272 ZY= 20.8228
XZ= -21.9325 YZ= 25.9908 ZZ= 162.3030
Eigenvalues: 46.9074 127.5355 174.3449
8 C Isotropic = 58.7535 Anisotropy = 117.8435
XX= 3.0617 YX= -19.5740 ZX= -46.6436
XY= -29.4541 YY= 52.1078 ZY= -0.1468
XZ= -42.8299 YZ= 4.4361 ZZ= 121.0910
Eigenvalues: -19.1766 58.1211 137.3158
9 C Isotropic = 75.8490 Anisotropy = 112.2451
XX= 44.4331 YX= -36.7515 ZX= -32.6338
XY= -30.9262 YY= 44.4481 ZY= 4.1146
XZ= -33.3503 YZ= 0.8554 ZZ= 138.6656
Eigenvalues: 6.8188 70.0490 150.6791
10 C Isotropic = 74.0934 Anisotropy = 81.5985
XX= 71.3063 YX= -33.3939 ZX= 31.4233
XY= -26.2754 YY= 44.2430 ZY= -7.7843
XZ= 29.8022 YZ= 1.3023 ZZ= 106.7310
Eigenvalues: 22.3923 71.3955 128.4925
11 Br Isotropic = 1896.9045 Anisotropy = 1580.7463
XX= 2567.8450 YX= 568.6165 ZX= 348.0435
XY= 587.3599 YY= 1709.1747 ZY= 148.3898
XZ= 344.9933 YZ= 149.3612 ZZ= 1413.6939
Eigenvalues: 1316.7191 1423.2591 2950.7354
12 C Isotropic = 22.5414 Anisotropy = 123.9623
XX= 8.2635 YX= -14.4809 ZX= 71.0352

XY= -34.3742 YY=   10.8200 ZY=   -5.5843
XZ=   65.4781 YZ= -15.0026 ZZ=   48.5407
Eigenvalues: -46.1293   8.5706 105.1830
 13 O   Isotropic = -59.3343   Anisotropy = 253.9822
XX= -50.5463 YX= -78.4798 ZX= 101.2402
XY= -79.1866 YY= -147.1928 ZY= -27.1735
XZ= 100.3209 YZ= -27.4012 ZZ=   19.7360
Eigenvalues: -195.3555 -92.6347 109.9872
 14 N   Isotropic = -130.5772   Anisotropy = 259.7023
XX= -123.3449 YX=   25.1259 ZX= 138.0213
XY=   39.1996 YY= -160.9567 ZY= -97.7183
XZ= 148.5933 YZ= -101.6291 ZZ= -107.4300
Eigenvalues: -316.0386 -118.2507   42.5577
 15 C   Isotropic =   26.1198   Anisotropy =   75.1599
XX=   22.3799 YX=   25.6313 ZX=   52.0869
XY=   41.1101 YY=   46.6147 ZY= -46.4159
XZ=   67.3882 YZ= -23.0426 ZZ=   9.3649
Eigenvalues: -64.9840   67.1171   76.2264
 16 C   Isotropic =   63.1574   Anisotropy = 103.0511
XX=   77.1225 YX=   0.2408 ZX=   45.9422
XY=   8.9621 YY=   28.5300 ZY= -34.7359
XZ=   48.4578 YZ= -28.1632 ZZ=   83.8196
Eigenvalues: 4.1341   53.4799 131.8581
 17 N   Isotropic =   99.0600   Anisotropy = 126.1939
XX= 113.3400 YX= -46.6423 ZX=   46.2159
XY= -51.1042 YY=   37.6635 ZY=   3.7523
XZ=   44.2436 YZ=   0.8896 ZZ= 146.1764
Eigenvalues: 9.7925 104.1982 183.1892
 18 C   Isotropic =   62.9802   Anisotropy = 120.1331
XX=   71.2161 YX=   14.3613 ZX=   64.2832
XY=   9.1705 YY=   39.7421 ZY= -35.1772
XZ=   64.9332 YZ= -39.2376 ZZ=   77.9824
Eigenvalues: -13.1591   59.0308 143.0689
 19 C   Isotropic =   70.9689   Anisotropy = 136.3564
XX=   59.8701 YX= -23.7909 ZX=   79.1915
XY= -20.3509 YY=   60.2209 ZY=   -9.6536
XZ=   80.0069 YZ=   -7.7636 ZZ=   92.8156
Eigenvalues: -7.0301   58.0636 161.8732
 20 C   Isotropic =   68.8568   Anisotropy = 145.8400
XX=   85.2866 YX= -25.4527 ZX=   59.6208
XY= -20.9396 YY=   3.4383 ZY= -25.0343
XZ=   52.2734 YZ= -19.8228 ZZ= 117.8456
Eigenvalues: -3.3388   43.8258 166.0835
 21 I   Isotropic = 3786.6412   Anisotropy = 2017.6949
XX= 3709.8100 YX= -798.3762 ZX= -574.0259
XY= -690.6544 YY= 3563.1629 ZY= 734.9348
XZ= -558.7298 YZ= 637.3734 ZZ= 4086.9506
Eigenvalues: 2865.3212 3362.8312 5131.7711
 22 H   Isotropic =   24.3216   Anisotropy =   9.8599
XX=   25.3034 YX=   4.0926 ZX=   2.1000
XY=   3.2320 YY=   28.2198 ZY=   -0.1014
XZ=   2.3636 YZ=   0.5947 ZZ=   19.4415
Eigenvalues: 18.5781   23.4917   30.8949
 23 H   Isotropic =   24.0938   Anisotropy =   9.9380
XX=   29.3508 YX=   -0.5299 ZX=   3.9663
XY=   -0.1355 YY=   23.8598 ZY=   -0.8906
XZ=   3.8494 YZ=   -0.8456 ZZ=   19.0708
Eigenvalues: 17.6707   23.8916   30.7191

24 H Isotropic = 24.3626 Anisotropy = 9.5311
XX= 28.5796 YX= 1.8045 ZX= 4.0391
XY= 0.6449 YY= 22.7719 ZY= 0.0298
XZ= 4.0097 YZ= 1.7305 ZZ= 21.7364
Eigenvalues: 19.8458 22.5254 30.7167
25 H Isotropic = 23.8386 Anisotropy = 9.5230
XX= 24.5959 YX= -0.2102 ZX= 2.4781
XY= 0.6158 YY= 29.8550 ZY= -2.1081
XZ= 2.1531 YZ= -2.0361 ZZ= 17.0650
Eigenvalues: 16.1043 25.2243 30.1873
26 H Isotropic = 24.4177 Anisotropy = 6.1409
XX= 24.3275 YX= 1.1819 ZX= -0.4105
XY= -0.1936 YY= 27.0423 ZY= -2.8866
XZ= 0.6118 YZ= -3.2524 ZZ= 21.8835
Eigenvalues: 20.4303 24.3113 28.5117
27 H Isotropic = 22.9710 Anisotropy = 7.1999
XX= 22.5999 YX= 2.3083 ZX= -5.1231
XY= 2.3434 YY= 26.5706 ZY= 1.4138
XZ= -4.9049 YZ= 1.6993 ZZ= 19.7424
Eigenvalues: 15.3315 25.8105 27.7709
28 H Isotropic = 24.7356 Anisotropy = 3.8870
XX= 24.2978 YX= 0.5998 ZX= -2.3526
XY= -0.1251 YY= 26.1672 ZY= 1.7076
XZ= -2.4245 YZ= 1.4537 ZZ= 23.7419
Eigenvalues: 21.2404 25.6395 27.3269
29 H Isotropic = 25.4558 Anisotropy = 4.2945
XX= 24.6875 YX= 0.0980 ZX= -1.9939
XY= 0.0405 YY= 26.2789 ZY= 1.5897
XZ= -2.2766 YZ= 2.1734 ZZ= 25.4010
Eigenvalues: 22.4143 25.6343 28.3188
30 H Isotropic = 25.6201 Anisotropy = 11.2476
XX= 24.0110 YX= -1.5181 ZX= -4.8139
XY= 0.3444 YY= 24.6812 ZY= 2.7577
XZ= -2.7969 YZ= 7.3775 ZZ= 28.1680
Eigenvalues: 20.0494 23.6923 33.1185

Isomer 10 (conformer 3)

1 C Isotropic = 58.5232 Anisotropy = 144.2261
XX= 20.9313 YX= 31.4356 ZX= -55.1555
XY= 35.2696 YY= 31.6849 ZY= 45.2592
XZ= -56.2999 YZ= 44.9759 ZZ= 122.9534
Eigenvalues: -39.1727 60.0684 154.6740
2 C Isotropic = 47.1843 Anisotropy = 112.4164
XX= -5.5131 YX= -46.4659 ZX= -32.3740
XY= -50.5237 YY= 38.0685 ZY= 4.7451
XZ= -33.5215 YZ= 5.0707 ZZ= 108.9975
Eigenvalues: -41.1739 60.5983 122.1286
3 C Isotropic = 70.2802 Anisotropy = 125.0017
XX= 71.0755 YX= -18.9900 ZX= -23.6511
XY= -24.8638 YY= 2.0476 ZY= 30.1205
XZ= -22.2955 YZ= 32.1041 ZZ= 137.7175
Eigenvalues: -8.4022 65.6281 153.6147
4 C Isotropic = 46.9340 Anisotropy = 144.4021
XX= 9.2526 YX= 16.2693 ZX= -50.1711
XY= 15.9450 YY= 16.0501 ZY= 37.4982
XZ= -52.4307 YZ= 38.3569 ZZ= 115.4995
Eigenvalues: -31.4743 29.0743 143.2021
5 C Isotropic = 56.7090 Anisotropy = 169.9060
XX= 15.3972 YX= -23.0031 ZX= -47.8193
XY= -25.5713 YY= 10.1184 ZY= 34.3321
XZ= -45.7241 YZ= 34.6440 ZZ= 144.6115
Eigenvalues: -12.0218 12.1692 169.9797
6 C Isotropic = 59.8072 Anisotropy = 174.4628
XX= 53.4691 YX= -6.7832 ZX= -39.8951
XY= -5.5612 YY= -23.6606 ZY= 53.6080
XZ= -34.6184 YZ= 52.7128 ZZ= 149.6131
Eigenvalues: -38.8749 42.1808 176.1157
7 N Isotropic = 116.9153 Anisotropy = 85.5468
XX= 129.8484 YX= 15.4040 ZX= -19.9686
XY= 8.7936 YY= 64.2341 ZY= 31.3891
XZ= -21.3112 YZ= 36.8925 ZZ= 156.6634
Eigenvalues: 48.9053 127.8941 173.9465
8 C Isotropic = 59.3968 Anisotropy = 117.4248
XX= -0.2936 YX= -29.7328 ZX= -39.3375
XY= -32.5805 YY= 57.8024 ZY= 9.8117
XZ= -43.4585 YZ= 8.0108 ZZ= 120.6816
Eigenvalues: -22.5046 63.0150 137.6800
9 C Isotropic = 75.6962 Anisotropy = 111.8048
XX= 44.1882 YX= -43.6635 ZX= -26.0045
XY= -35.7215 YY= 45.2399 ZY= 15.8762
XZ= -25.2442 YZ= 12.9036 ZZ= 137.6606
Eigenvalues: 4.4814 72.3746 150.2327
10 C Isotropic = 73.5194 Anisotropy = 80.3346
XX= 86.3180 YX= -12.4570 ZX= 28.7147
XY= -20.8232 YY= 27.7107 ZY= -11.4036
XZ= 19.5642 YZ= -16.9899 ZZ= 106.5297
Eigenvalues: 22.5359 70.9466 127.0759
11 Br Isotropic = 1895.8608 Anisotropy = 1583.6436
XX= 2557.8495 YX= 599.5388 ZX= 276.9791
XY= 633.7629 YY= 1734.8136 ZY= 114.1468
XZ= 304.7534 YZ= 135.8621 ZZ= 1394.9193
Eigenvalues: 1322.5297 1413.4295 2951.6232
12 C Isotropic = 22.4919 Anisotropy = 122.2113
XX= 40.7486 YX= -12.6658 ZX= 49.1794

XY= 9.8794 YY= -20.7435 ZY= -45.7411
XZ= 54.8701 YZ= -34.5691 ZZ= 47.4706
Eigenvalues: -45.7350 9.2446 103.9661
13 O Isotropic = -60.1218 Anisotropy = 253.3051
XX= -18.1292 YX= -54.5444 ZX= 89.1816
XY= -53.5564 YY= -177.5412 ZY= -42.5550
XZ= 96.9734 YZ= -40.9187 ZZ= 15.3051
Eigenvalues: -195.1431 -93.9704 108.7483
14 N Isotropic = -130.9279 Anisotropy = 260.6930
XX= -161.5185 YX= 2.7432 ZX= 166.1019
XY= -6.4644 YY= -116.1805 ZY= -42.4269
XZ= 177.6387 YZ= -46.8547 ZZ= -115.0848
Eigenvalues: -315.7244 -119.9268 42.8674
15 C Isotropic = 26.0131 Anisotropy = 82.3887
XX= 7.7257 YX= 30.4539 ZX= 70.2238
XY= 10.6372 YY= 56.2346 ZY= -17.6499
XZ= 66.4717 YZ= -35.9215 ZZ= 14.0790
Eigenvalues: -66.5918 63.6921 80.9389
16 C Isotropic = 62.3084 Anisotropy = 102.2928
XX= 52.5476 YX= -14.0419 ZX= 60.2249
XY= -22.5996 YY= 56.3606 ZY= -7.0837
XZ= 57.9451 YZ= -11.5367 ZZ= 78.0169
Eigenvalues: 3.4290 52.9926 130.5036
17 N Isotropic = 97.8581 Anisotropy = 127.6998
XX= 122.7301 YX= -41.8726 ZX= 36.0665
XY= -39.3523 YY= 23.8323 ZY= -22.6608
XZ= 34.7440 YZ= -19.0655 ZZ= 147.0119
Eigenvalues: 8.8190 101.7640 182.9913
18 C Isotropic = 62.8583 Anisotropy = 120.1646
XX= 52.3488 YX= -11.6406 ZX= 71.6743
XY= -6.5200 YY= 64.2324 ZY= -22.4103
XZ= 76.8456 YZ= -18.8369 ZZ= 71.9938
Eigenvalues: -13.3496 58.9565 142.9681
19 C Isotropic = 71.6277 Anisotropy = 135.3746
XX= 90.9658 YX= 4.2355 ZX= 61.3176
XY= -0.2581 YY= 29.4456 ZY= -46.3813
XZ= 60.5137 YZ= -46.3846 ZZ= 94.4717
Eigenvalues: -6.5859 59.5916 161.8774
20 C Isotropic = 72.1536 Anisotropy = 141.0314
XX= 72.1220 YX= -32.5354 ZX= 68.3182
XY= -42.5138 YY= 24.5841 ZY= -12.8361
XZ= 51.4338 YZ= -4.2276 ZZ= 119.7548
Eigenvalues: -1.3226 51.6089 166.1746
21 I Isotropic = 3763.7325 Anisotropy = 2020.2439
XX= 4282.1315 YX= -297.1616 ZX= -852.0197
XY= -330.0999 YY= 2849.7759 ZY= 89.3542
XZ= -857.9561 YZ= 31.4764 ZZ= 4159.2902
Eigenvalues: 2769.6673 3410.9685 5110.5618
22 H Isotropic = 24.2028 Anisotropy = 10.0944
XX= 25.1417 YX= 4.2912 ZX= 1.6957
XY= 3.6873 YY= 28.1435 ZY= -0.8339
XZ= 2.2838 YZ= -0.5745 ZZ= 19.3232
Eigenvalues: 18.2858 23.3903 30.9324
23 H Isotropic = 24.0631 Anisotropy = 9.7417
XX= 29.1455 YX= -0.2170 ZX= 3.9978
XY= 0.2107 YY= 23.7796 ZY= -1.1866
XZ= 3.9029 YZ= -1.3578 ZZ= 19.2642
Eigenvalues: 17.6440 23.9876 30.5575

24 H Isotropic = 23.9680 Anisotropy = 10.1937
XX= 27.5217 YX= 1.8748 ZX= 3.9601
XY= 1.3995 YY= 22.1535 ZY= 1.3994
XZ= 5.2305 YZ= 1.8936 ZZ= 22.2289
Eigenvalues: 19.4110 21.7292 30.7639
25 H Isotropic = 23.7886 Anisotropy = 10.0386
XX= 24.2930 YX= -0.5567 ZX= 2.6805
XY= 0.5519 YY= 29.6710 ZY= -2.9721
XZ= 2.0080 YZ= -3.3110 ZZ= 17.4018
Eigenvalues: 16.0155 24.8693 30.4810
26 H Isotropic = 24.2830 Anisotropy = 5.6110
XX= 24.1932 YX= 0.3729 ZX= 0.2320
XY= -0.5236 YY= 27.2601 ZY= -2.0532
XZ= 0.3936 YZ= -2.4209 ZZ= 21.3958
Eigenvalues: 20.6191 24.2062 28.0237
27 H Isotropic = 23.0251 Anisotropy = 7.0887
XX= 22.2080 YX= 2.0574 ZX= -4.6857
XY= 1.9572 YY= 26.9641 ZY= 2.2670
XZ= -4.9328 YZ= 2.1542 ZZ= 19.9030
Eigenvalues: 15.3461 25.9782 27.7509
28 H Isotropic = 24.6856 Anisotropy = 3.7510
XX= 25.0147 YX= 0.3497 ZX= -2.8612
XY= 1.0219 YY= 25.4089 ZY= 0.5472
XZ= -2.6874 YZ= 0.9727 ZZ= 23.6331
Eigenvalues: 21.2161 25.6543 27.1862
29 H Isotropic = 25.3603 Anisotropy = 3.7204
XX= 25.5612 YX= 0.5333 ZX= -2.2486
XY= 0.5566 YY= 25.6854 ZY= 0.5795
XZ= -2.9829 YZ= 0.8633 ZZ= 24.8343
Eigenvalues: 22.3154 25.9249 27.8406
30 H Isotropic = 24.7633 Anisotropy = 11.7749
XX= 26.3025 YX= -0.9852 ZX= -5.8514
XY= -1.5595 YY= 23.6705 ZY= 1.7368
XZ= -8.1678 YZ= -0.3516 ZZ= 24.3170
Eigenvalues: 18.2120 23.4647 32.6133

Isomer 10 (conformer 4)

1 C Isotropic = 58.2957 Anisotropy = 144.0363
XX= 72.5426 YX= 12.5053 ZX= 75.1629
XY= 15.6166 YY= 32.3347 ZY= -55.0402
XZ= 76.3421 YZ= -53.2415 ZZ= 70.0099
Eigenvalues: -39.3045 59.8717 154.3199
2 C Isotropic = 47.2413 Anisotropy = 112.9440
XX= 32.5553 YX= -45.6691 ZX= 62.9541
XY= -49.2575 YY= 37.9446 ZY= 14.3341
XZ= 63.5974 YZ= 12.1184 ZZ= 71.2241
Eigenvalues: -41.5735 60.7602 122.5373
3 C Isotropic = 69.9535 Anisotropy = 124.7652
XX= 95.8242 YX= -29.1441 ZX= 40.0390
XY= -34.2514 YY= 1.8958 ZY= -19.7027
XZ= 38.7046 YZ= -23.0840 ZZ= 112.1405
Eigenvalues: -8.5703 65.3005 153.1303
4 C Isotropic = 46.7100 Anisotropy = 144.2674
XX= 58.0522 YX= 0.6531 ZX= 72.7740
XY= 0.8328 YY= 16.5812 ZY= -41.2169
XZ= 74.7121 YZ= -42.0178 ZZ= 65.4966
Eigenvalues: -31.8351 29.0768 142.8882
5 C Isotropic = 56.4594 Anisotropy = 169.5406
XX= 63.8077 YX= -35.3491 ZX= 78.8211
XY= -36.7045 YY= 10.6994 ZY= -23.0206
XZ= 76.6446 YZ= -25.0700 ZZ= 94.8711
Eigenvalues: -12.2559 12.1477 169.4865
6 C Isotropic = 60.3371 Anisotropy = 174.1588
XX= 92.6642 YX= -26.6811 ZX= 62.1104
XY= -24.9264 YY= -22.2813 ZY= -48.3549
XZ= 57.4372 YZ= -47.7885 ZZ= 110.6284
Eigenvalues: -38.2032 42.7715 176.4430
7 N Isotropic = 116.9351 Anisotropy = 85.3476
XX= 147.7776 YX= 1.3509 ZX= 23.4516
XY= -3.0542 YY= 64.5561 ZY= -33.3831
XZ= 24.9019 YZ= -40.2020 ZZ= 138.4717
Eigenvalues: 48.6088 128.3630 173.8336
8 C Isotropic = 59.6020 Anisotropy = 117.1605
XX= 43.5963 YX= -31.0532 ZX= 69.2514
XY= -34.7336 YY= 58.0973 ZY= 3.0420
XZ= 72.8160 YZ= 2.9957 ZZ= 77.1124
Eigenvalues: -22.3920 63.4889 137.7090
9 C Isotropic = 75.4627 Anisotropy = 112.5535
XX= 72.5562 YX= -46.8585 ZX= 51.1032
XY= -39.1957 YY= 45.7978 ZY= -2.5126
XZ= 50.6661 YZ= 3.9833 ZZ= 108.0341
Eigenvalues: 3.4046 72.4852 150.4983
10 C Isotropic = 73.8897 Anisotropy = 80.1319
XX= 73.9405 YX= -5.4646 ZX= -16.2717
XY= -15.5291 YY= 27.8346 ZY= 18.0803
XZ= -7.3707 YZ= 20.5102 ZZ= 119.8942
Eigenvalues: 22.6720 71.6863 127.3110
11 Br Isotropic = 1897.0446 Anisotropy = 1575.1774
XX= 2209.9171 YX= 518.3647 ZX= -600.3242
XY= 544.4621 YY= 1739.2843 ZY= -333.3890
XZ= -606.0758 YZ= -329.3918 ZZ= 1741.9324
Eigenvalues: 1322.7161 1421.2548 2947.1628
12 C Isotropic = 22.3639 Anisotropy = 123.1391
XX= 7.5688 YX= -0.0165 ZX= -34.6976

XY= 24.2270 YY= -21.4307 ZY= 39.8522
XZ= -39.5672 YZ= 37.3445 ZZ= 80.9535
Eigenvalues: -45.9876 8.6226 104.4566
13 O Isotropic = -60.0754 Anisotropy = 252.6535
XX= -73.9322 YX= -37.5695 ZX= -55.6894
XY= -34.9601 YY= -177.4438 ZY= 58.0174
XZ= -63.9825 YZ= 58.1005 ZZ= 71.1498
Eigenvalues: -195.1076 -93.4789 108.3602
14 N Isotropic = -130.9312 Anisotropy = 260.4593
XX= -268.1888 YX= 18.0709 ZX= -109.7322
XY= 8.9395 YY= -115.6312 ZY= 42.1198
XZ= -119.4050 YZ= 45.1045 ZZ= -8.9735
Eigenvalues: -315.5828 -119.9191 42.7084
15 C Isotropic = 26.0096 Anisotropy = 82.7387
XX= -36.8501 YX= 40.4249 ZX= -51.8353
XY= 16.4674 YY= 56.4990 ZY= 12.7989
XZ= -47.3295 YZ= 22.9146 ZZ= 58.3800
Eigenvalues: -66.9072 63.7674 81.1687
16 C Isotropic = 62.2710 Anisotropy = 102.3033
XX= 18.5871 YX= -9.0669 ZX= -38.9565
XY= -18.6293 YY= 55.3112 ZY= 12.8274
XZ= -37.3723 YZ= 14.2495 ZZ= 112.9147
Eigenvalues: 3.6001 52.7397 130.4732
17 N Isotropic = 97.8753 Anisotropy = 127.4901
XX= 104.6320 YX= -31.4558 ZX= -21.0301
XY= -27.8196 YY= 21.8094 ZY= 31.4640
XZ= -21.4835 YZ= 29.4931 ZZ= 167.1846
Eigenvalues: 8.9135 101.8437 182.8687
18 C Isotropic = 63.1341 Anisotropy = 119.9843
XX= 7.9582 YX= -4.1217 ZX= -48.8742
XY= 1.6851 YY= 63.5809 ZY= 21.5775
XZ= -54.2504 YZ= 19.6661 ZZ= 117.8631
Eigenvalues: -13.0075 59.2861 143.1236
19 C Isotropic = 71.7972 Anisotropy = 135.1267
XX= 52.0948 YX= 20.6850 ZX= -46.3871
XY= 17.0368 YY= 28.3872 ZY= 41.3529
XZ= -44.2679 YZ= 39.8146 ZZ= 134.9095
Eigenvalues: -6.3937 59.9036 161.8817
20 C Isotropic = 72.1641 Anisotropy = 141.1863
XX= 40.5767 YX= -28.7563 ZX= -40.1986
XY= -34.8723 YY= 22.7982 ZY= 23.6988
XZ= -23.7048 YZ= 12.4340 ZZ= 153.1174
Eigenvalues: -1.5255 51.7294 166.2883
21 I Isotropic = 3723.6289 Anisotropy = 2066.5348
XX= 4802.6967 YX= -251.2309 ZX= 634.7777
XY= -321.8899 YY= 2830.8730 ZY= -9.5987
XZ= 642.4356 YZ= -22.9790 ZZ= 3537.3171
Eigenvalues: 2780.3536 3289.2144 5101.3188
22 H Isotropic = 24.2443 Anisotropy = 10.0373
XX= 23.1160 YX= 4.2671 ZX= -3.0542
XY= 3.7324 YY= 28.1431 ZY= -0.5366
XZ= -3.7018 YZ= -0.8976 ZZ= 21.4738
Eigenvalues: 18.3657 23.4314 30.9359
23 H Isotropic = 24.0962 Anisotropy = 9.7096
XX= 25.1548 YX= 0.2514 ZX= -6.2548
XY= 0.6828 YY= 23.7705 ZY= 1.0270
XZ= -6.1878 YZ= 1.2938 ZZ= 23.3633
Eigenvalues: 17.7410 23.9783 30.5692

24 H Isotropic = 24.0219 Anisotropy = 10.2298
XX= 23.9110 YX= 1.1790 ZX= -4.5869
XY= 0.8507 YY= 22.3286 ZY= -1.6588
XZ= -6.0879 YZ= -2.2821 ZZ= 25.8260
Eigenvalues: 19.3532 21.8707 30.8418
25 H Isotropic = 23.8282 Anisotropy = 9.9772
XX= 21.7686 YX= 0.7406 ZX= -4.3236
XY= 1.6059 YY= 29.6066 ZY= 2.6658
XZ= -3.6854 YZ= 3.3523 ZZ= 20.1096
Eigenvalues: 16.1419 24.8631 30.4797
26 H Isotropic = 24.3457 Anisotropy = 5.6422
XX= 23.5530 YX= 1.0828 ZX= -1.1859
XY= 0.0591 YY= 27.2392 ZY= 2.2096
XZ= -1.1851 YZ= 2.2936 ZZ= 22.2448
Eigenvalues: 20.7628 24.1670 28.1071
27 H Isotropic = 23.0169 Anisotropy = 7.1038
XX= 24.9568 YX= 1.1109 ZX= 2.8983
XY= 0.9950 YY= 27.1077 ZY= -2.5956
XZ= 3.2266 YZ= -2.4258 ZZ= 16.9863
Eigenvalues: 15.3196 25.9784 27.7528
28 H Isotropic = 24.7038 Anisotropy = 3.7654
XX= 26.6690 YX= -0.0094 ZX= 1.7953
XY= 0.7536 YY= 25.4313 ZY= -0.7658
XZ= 1.5571 YZ= -0.9839 ZZ= 22.0109
Eigenvalues: 21.2557 25.6416 27.2140
29 H Isotropic = 25.3569 Anisotropy = 3.7104
XX= 27.1324 YX= 0.1720 ZX= 1.3880
XY= 0.3080 YY= 25.7149 ZY= -0.6608
XZ= 2.1904 YZ= -0.9842 ZZ= 23.2232
Eigenvalues: 22.3137 25.9264 27.8304
30 H Isotropic = 24.8633 Anisotropy = 11.6367
XX= 30.7043 YX= -0.7935 ZX= 3.3829
XY= -2.0440 YY= 23.7835 ZY= -1.0210
XZ= 5.7532 YZ= 0.6527 ZZ= 20.1020
Eigenvalues: 18.3857 23.5831 32.6211

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