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Supporting Information

Long-Range Residual Dipolar Couplings: A Tool for Determining the Configuration of Small Molecules

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NMR experiments:

All experiments for the isotropic and anisotropic NMR measurements were performed at 298 K on a Bruker 900 MHz NMR spectrometer operating at 900.01 MHz ^{1}H frequency and equipped with a triple resonance TCI-cryo probe. All spectra were recorded at 25°C. Selective spectra were acquired as a 32*(t_1)×16384*(t_2) data matrices, where N* refers to N complex pairs, using 64 transients per FID and a 2 s delay between scans. Spectral widths of 37000 Hz and 20 Hz were chosen in the direct and indirect dimensions, respectively. The time domain data was processed by zero filling to 32 k and 16 k points in the ω_2 and ω_1 dimensions respectively, with a sine square bell window function in both dimensions.

The CLIP-HSQC experiment was carried out to extract total coupling constants ($^1T_{CH}$) and scalar coupling constants ($^1J_{CH}$) and the INEPT delay used corresponds to an average coupling constant of 145 Hz. The spectrum was acquired with 512*(t_1)×8192*(t_2) data points with spectral widths in direct and indirect dimensions of 10 ppm and 20 ppm, respectively. The spectra were processed with squared sine bell window function in both dimensions and zero filled by a factor of two in ω_2 and a factor of four in ω_1. For each coupling the corresponding traces of the CLIP-HSQC spectra were extracted, subjected to an inverse Fourier transformation and processed by zero filling to 32 k points.

Sample preparation:

The alignment of the molecule was achieved by reversible compression and relaxation of poly-methyl methacrylate (PMMA) gel.[1] $CDCl_3$ (400 μL) was added to a 5 mm NMR tube with a dried 25 mm long polymer stick and was allowed to swell solely in the radial direction by blocking the vertical expansion using a plunger. Swelling of the gel was observed by monitoring the ^2D quadrupolar splitting of the solvent signal. After 15-24 h the gel was equilibrated, resulting in a splitting of 51 Hz. The gel was then washed with solvent several times to remove residual monomers and a solution of **1 (**12 mg of **1** dissolved in 300 μL $CDCl_3$) was added. RDCs were measured when the gels were fully compressed. For the isotropic measurement, 8 mg of **1** was dissolved in 400 μL $CDCl_3$.

Selective inversion of multiple protons:

One of the advantages of the experiment is the selective inversion of several protons not coupled to a common carbon for the extraction of the LR RDCs. Generally, the heteronuclear *J*-coupling between atoms connected by more than three bonds is not observable in solution-state NMR. In knowing the constitution of the molecule, the coupling network can be anticipated and those nuclei that can be multiplexed, i.e. those that do not share a carbon as coupling partner, can be selected. In the rare cases that a dipolar coupling is observed in the absence of a *J*-coupling, this can easily be identified from the more complicated multiplicity pattern in ω_1 which is expected then to deviate from a doublet. Figure S1(c) presents the inversion of the proton H22 and H12 performed simultaneously by using the 1D single pulsed-field-gradient echo (SPFGE) scheme, in which a selective 180° pulse is applied to both protons. The multiplexed 2D spectrum, when H22 and H12 were inverted together, is presented in Figure 3 in the main text. The spectrum enables the extraction of several multiple bond CH couplings. Some of the cross peaks are shown on the top of 2D plot for better clarity, and overlay of cross peaks both in isotropic and anisotropic phases are shown side-by-side.

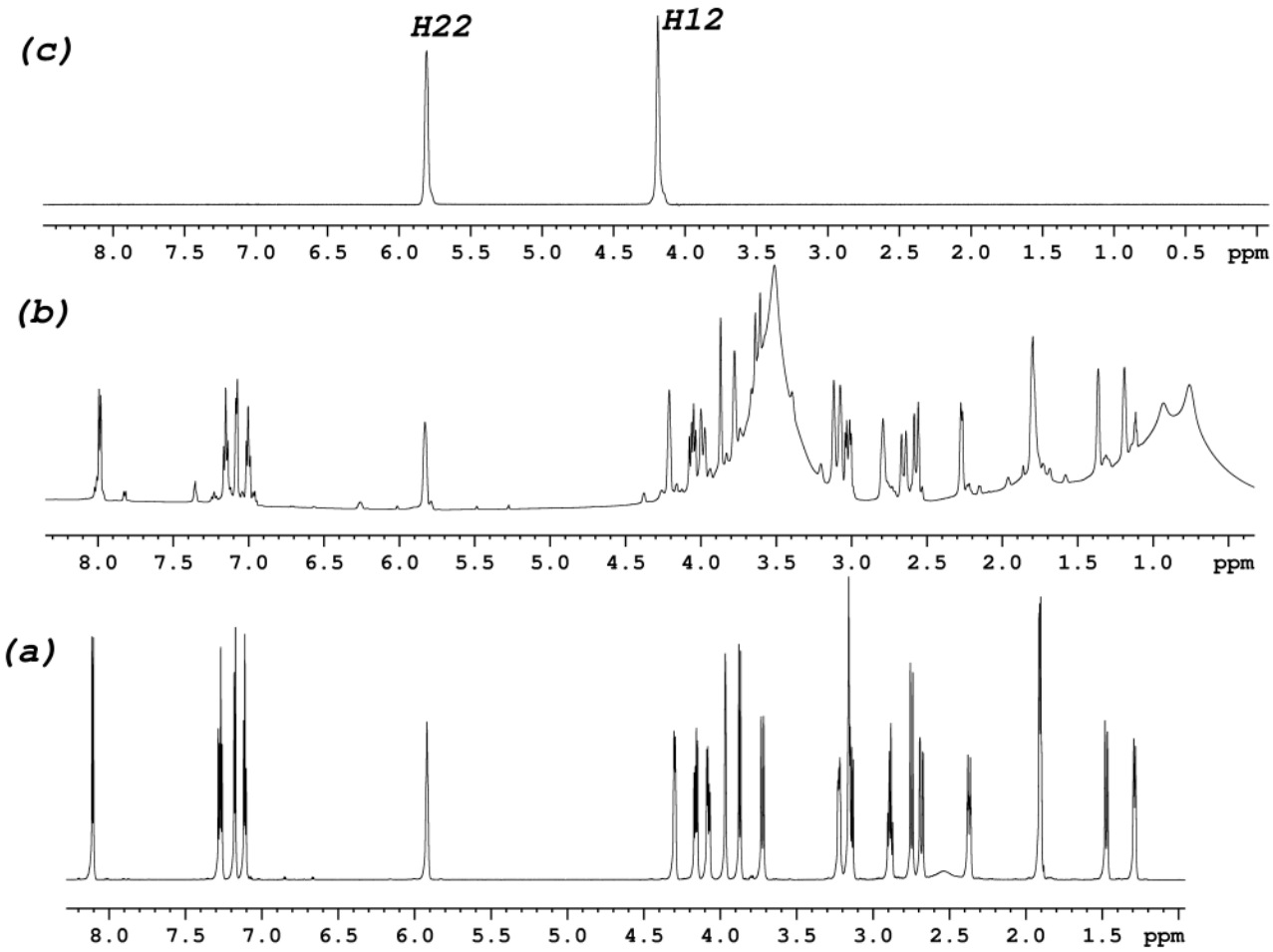


Figure S1: 1D proton spectrum of strychnine, (a) in isotropic phase, (b) in anisotropic phase and (c) in anisotropic phase when the protons H22 and H12 were simultaneously inverted. The multiplexing spectra for these two protons are provided in the main text.

Sensitivity and resolution:

Generally, when the detection is on the carbon instead of proton, the sensitivity of the experiment is eight times lower.[2] However, there is an effect from the ^{1}H-^{1}H dipolar couplings present during the direct detection dimension for an anisotropic sample. The effect depends on the number of dipolar-coupled protons and therefore is difficult to predict. Yet it can be measured experimentally. The ^{1}H-^{1}H dipolar couplings are present in the direct detection dimension of proton detected experiments, for example as in the SJS-HSQC experiment.[3] The presence of these homonuclear dipolar couplings in direct detection causes dipolar broadening with consequential loss in sensitivity. The dipolar broadening is greater when the proton of interest is coupled to many other protons. On the other hand, for the ^{13}C detected experiment presented in this paper the ^{1}H-^{1}H dipolar couplings along with ^{13}C-^{1}H dipolar couplings are removed during the detection period and only the chemical shifts are observed. The absence of line broadening caused by dipolar couplings during the detection period improves the sensitivity of the experiment over the general sensitivity ratio of carbon detected versus proton detected experiments of $(\gamma_C/\gamma_H)^{3/2} = 1/8$. We performed sensitivity comparison experiments between our method and SJS-HSQC for few protons, namely, H12, H15a, H15b and H22 and the ratio of signal-to-noise ratios (our method vs. SJS-HSQC) are given for these protons in the Table S1. As one can see, the signal-to-noise ratios are at the order of 0.8 to 0.9 and thus much larger than the 1/8 expected from the comparison of the gyromagnetic ratios indicating that removal of the ^{1}H-^{1}H dipolar couplings has a large beneficial effect on the S/N of our experiment. We also found that both techniques returned the same coupling values, and the *J*-couplings measured using the new experiment are similar to the reported data.[4] Importantly, despite the slightly lower sensitivity, the new experiment allows the *J*-coupling to be measured to the same precision as in the SJS-HSQC experiment – the measured *J* errors for both experiments are the same (Table S1).

Table S1. Comparison of sensitivity and precision between the new experiment and the SJS-HSQC for a few selected CH pairs in strychnine. The second column represents the ratio of signal-to-noise ratios of present method and SJS-HSQC, and the third and fourth columns are the *J*-couplings and errors extracted from these methods. Statistics were calculated by superimposing 10 random strips of experimental noise over the peaks.

Correlation	"S/N (Our method)" / "S/N (SJS-HSQC)"	*J*-coupling	
		Our method	SJS-HSQC
C23-H22	0.82	7.04 ± 0.011	7.10 ± 0.010
C14-H22	0.84	8.83 ± 0.014	8.88 ± 0.012
C20-H22	0.78	5.94 ± 0.011	5.90 ± 0.013
C13-H15a	0.89	3.56 ± 0.050	3.60 ± 0.060
C14-H15b	0.93	7.98 ± 0.017	8.05 ± 0.015
C11-H12	0.82	6.86 ± 0.028	6.91 ± 0.025
C8-H12	0.86	5.67 ± 0.047	5.73 ± 0.052

Switching from a low field to a high field spectrometer, say from 500 MHz to 900 MHz, theoretically there will a sensitivity gain of 2.48 as the sensitivity depends on $B^{3/2}$, where B is the field strength. The measured S/N values for strychnine cross peaks range from 25 to 45. For a reduction of the field from 900 MHz to 500 MHz, the S/N range should decrease to 10.3-18.6. The experiment is therefore expected to work well at lower fields. The lower field will have a lower resolution, but as we detect ^{13}C in the direct dimension and ^{13}C chemical shift covers a much larger range (0-250 ppm), the resolution is not an issue at lower field.

Computational details:

Strychnine has six chiral centers whose different permutations leads to 64 different configurations or diastereomers. Since we focus on relative configuration, we set the absolute configuration at C7 to the naturally occurring *R*, resulting in 32 configurations. Each configuration was named after the configuration at carbons C5, C7, C8, C9, C16 and C23, i.e. *RRRRRR* indicates that all stereocenters at the indicated carbons have the *R* configuration. The X-ray crystallographic structure of strychnine was used as a starting point. The hydrogen positions were optimized by DFT at B3LYP/6-311+g(2d,p) level using Gaussian 09[5] using the ICF-PCM solvent continuum model with $CHCl_3$ as a solvent. Thus, accurate interatomic distances and orientations of CH vectors were obtained.[6] The structural models of the other 31 configurations were manually built from this DFT-optimized structure and were further optimized at the same level of DFT. Only 18 configurations, including the correct one, yielded energetically feasible structures and hence were used in the analysis. This was expected since the multicyclic constitution is not compatible with all configurations.

Cross-validation of one-bond and long range RDCs:

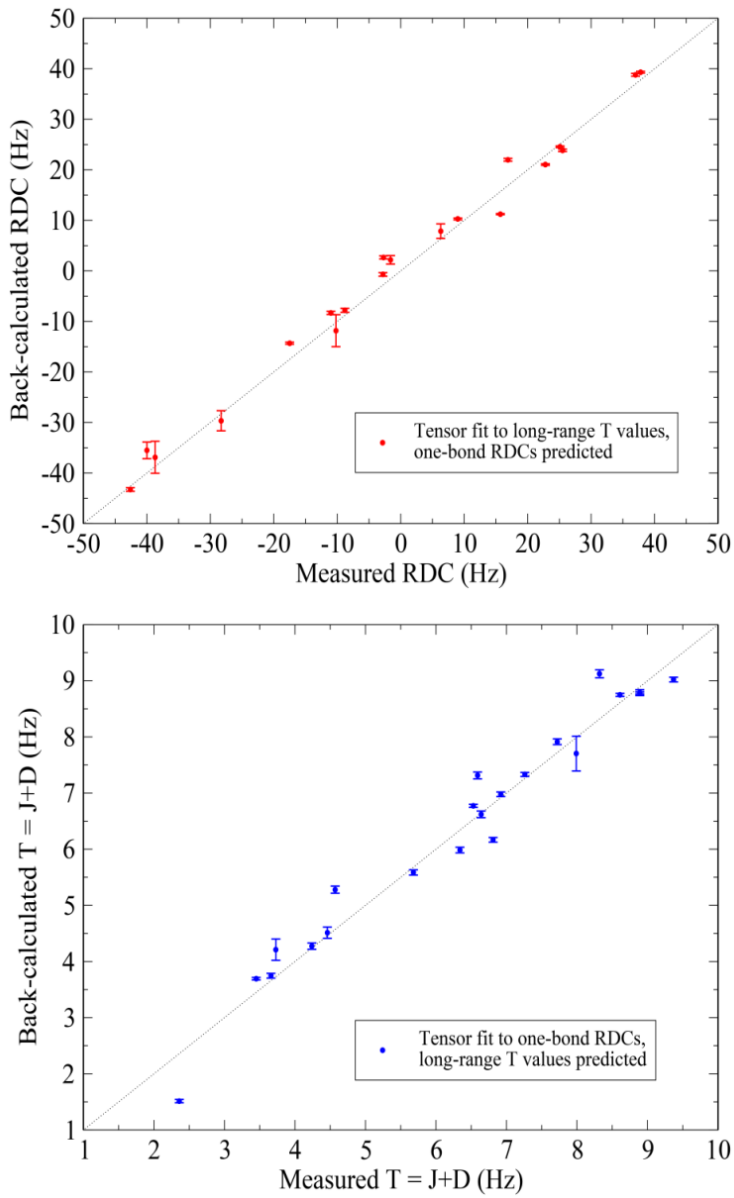


Figure S2. Cross-validation plots for the correct strychnine configuration of *SRRSRS*. (a) Correlation plot of experimental versus back-calculated LR RDCs; (b) Correlation plot of experimental versus back-calculated one-bond RDCs. Note that for an unknown configuration, such plots cannot be employed for determining if there are errors in the input data. These plots demonstrate the quality of the measured long range absolute ${}^{n}T_{CH}$ value.

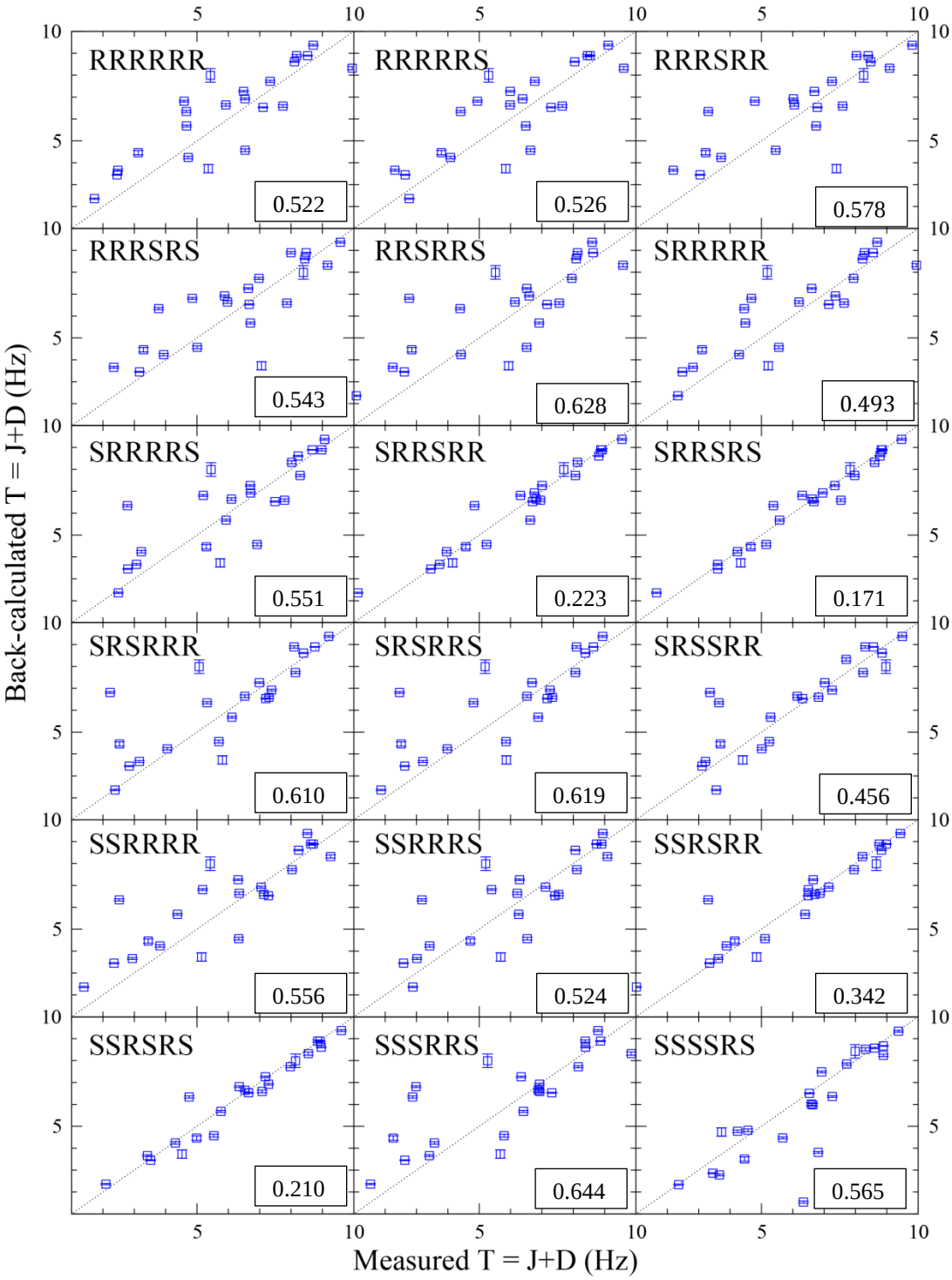


Figure S3: Correlation plots of the back-calculated vs. experimental absolute *T* values (*J*+*D*) for the eighteen DFT optimized strychnine configurations when only long range couplings are utilized. *Q* factors for the fits are shown in the boxes.

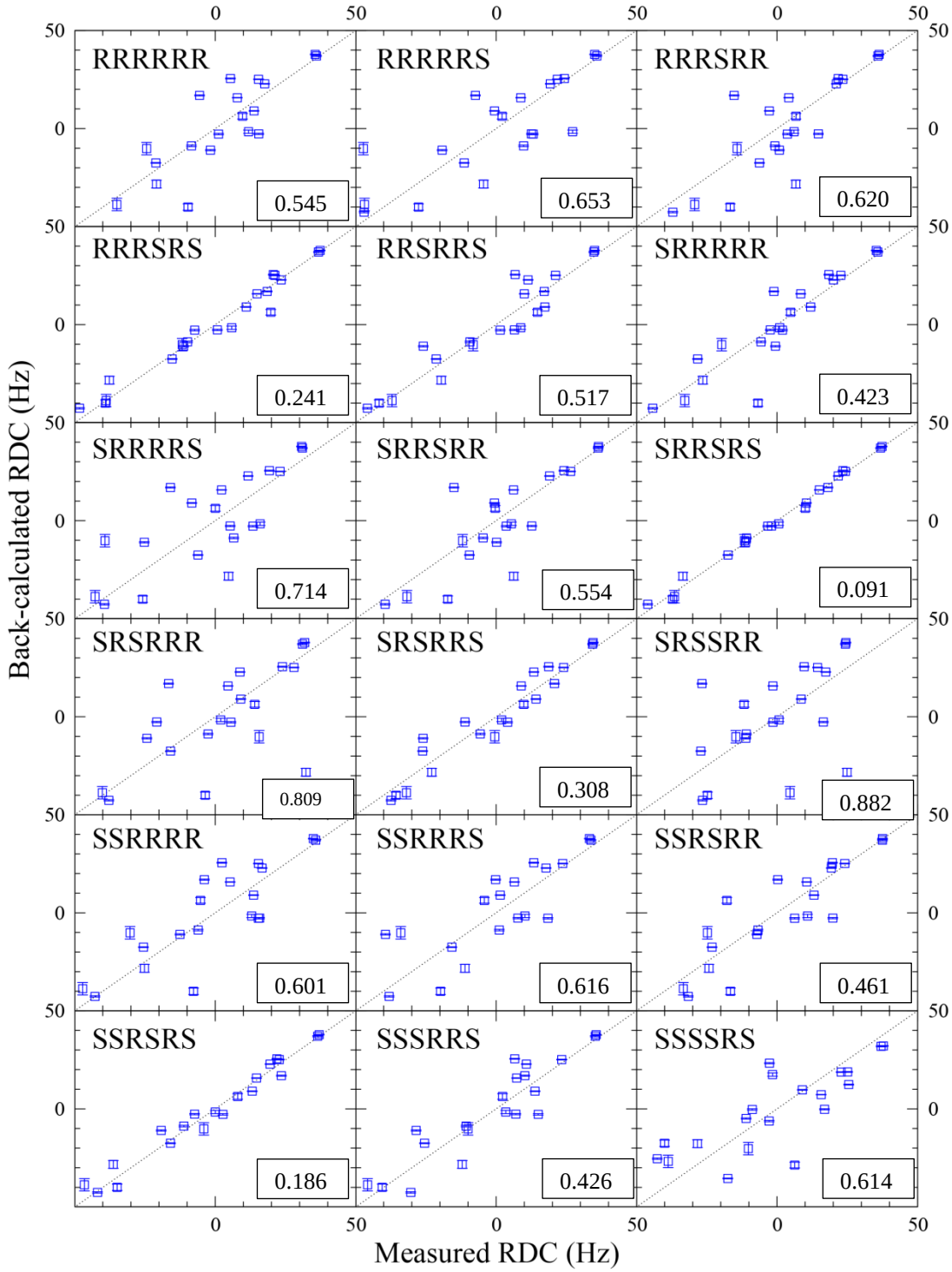


Figure S4: Correlation of plots of the back-calculated vs. experimental RDCs for the eighteen DFT optimized strychnine configurations when both one-bond and long range couplings are utilized. *Q* factors for the fits are shown in the boxes.

Assignment of diastereotopic protons:

Residual dipolar couplings have been successfully employed for the assignment of diastereotopic protons.[7] Herein, one-bond RDCs were used to distinguish between the two diastereotopic protons attached to C6, C18, C19, C22 and C24 which results in 32 possible combinations. The carbon for which the protons are swapped is marked with an asterisk. For example when protons on C24 are wrongly assigned for the configuration "6,18,19,22,24" then the *Q* factor rises from 0.074 to 0.508. From the plot of the *Q* factor for the different combinations of diastereotopic proton, it is clear that all combinations except for the two in which the C19 protons have been interchanged have higher *Q* factors. This indicates that the proton assignments are incorrect. On the other hand the two combinations in which the C19 protons have been interchanged (6,18,19,22,24 and 6,18,19*,22,24) have identical *Q* factors. When the protons on all other carbons are interchanged, the *Q* factors increase. Using this strategy, the eight diastereotopic protons can be unambiguously assigned. However, the proton pair at C19 was assigned using isotropic NMR restraints (NOESY).

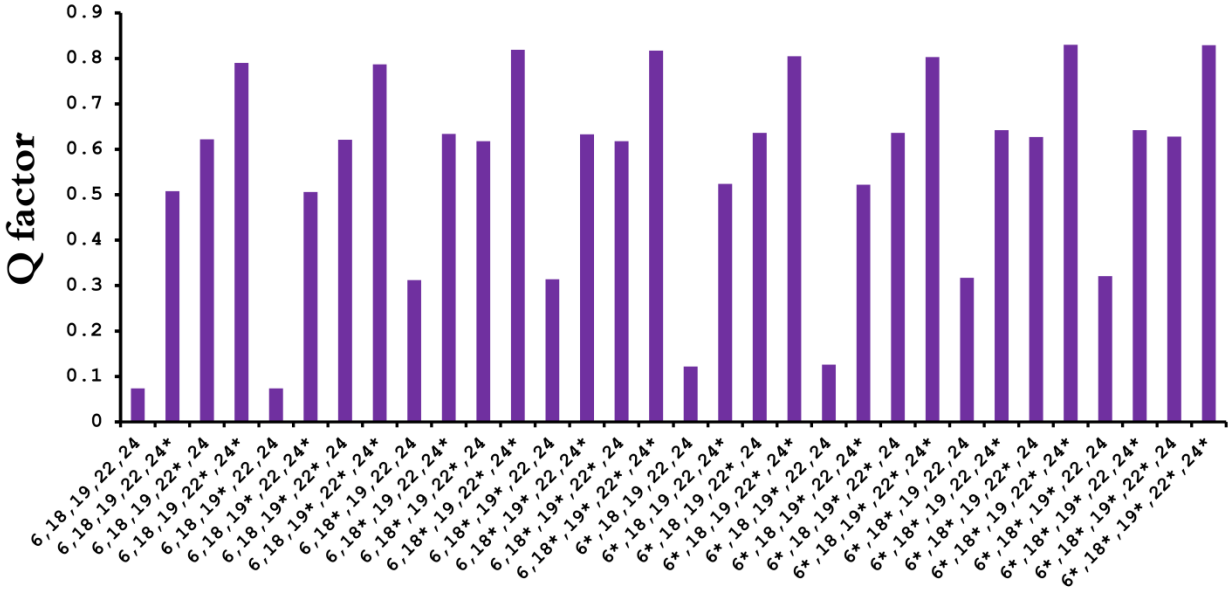


Figure S5: *Q* factors used in the assignment of the diastereotopic protons via 32 possible different combinations.

Determination of relative configuration:

Strychnine has six stereogenic centers, inverting each leads to 64 different configurations. Excluding enantiomers only 32 configurations are left. The natural stereochemistry of the C7 is assumed to be *R* and relative configurations of the adjacent stereogenic pairs can be determined from the *J*-couplings. From the *J*-coupling analysis, it is possible to determine relative configurations of adjacent stereogenic centers. The $^{3}J_{HH}$ for the proton pair H8/H13 is large (10.5 Hz) and hence the relative configuration for C8/C13 is anti. Consequently, the relative configuration of C13/C12 is either *SR* or *RS*. The proton H13 has a small coupling (3.1 Hz) to both protons H12 and H14 suggesting syn arrangements for both C13/C14 and C13/C12. Proton H13 also has a gauche coupling to carbon C15. Using the $^{3}J_{HH}$ and $^{3}J_{CH}$ couplings enables the relative configuration for C13/C14 to be restricted to *RR* or *SS*. Proton H12 has a small coupling to C11 (2.2 Hz) and a medium coupling (5.7 Hz) to C8. Thus, the relative configuration of the C13/C12 is either *RS* or *SR*. The Newman projections for C8/C13, C13/C14 and C12/C13 are presented in Figure S6.

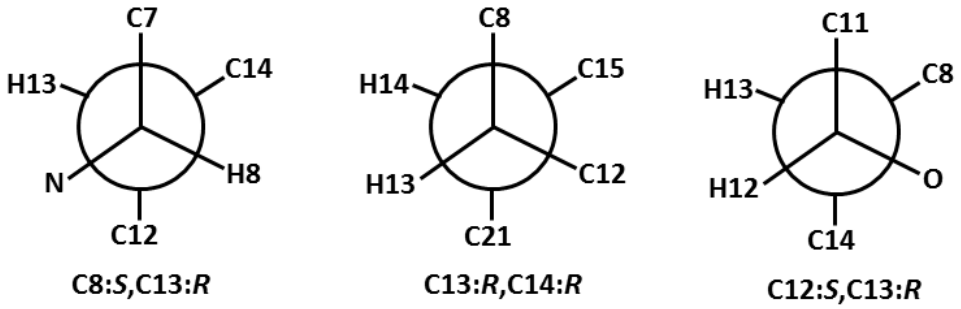


Figure S6: Newman projections for C8/C13, C13/C14 and C12/C13 dihedral derived from *J*-coupling analysis.

Table S2. Experimental one-bond $^1J_{CH}$ couplings, total couplings ($^1T_{CH}$) and errors[a].

Spin-pair	$^1T_{CH}$=$^1J_{CH}$+$^1D_{CH}$ (Hz)	error	$^1J_{CH}$ (Hz)	error
C16-H16	173.2	0.17	148.1	0.12
C15-H15a	136.0	1.44	129.7	0.14
C15-H15b	129.2	0.83	130.8	0.24
C14-H14	92.1	3.16	130.8	0.08
C13-H13	113.8	0.32	124.8	0.06
C8-H8	127.4	0.21	144.9	0.007
C4-H4	205.9	0.17	168.1	0.04
C3-H3	174.3	0.11	158.6	0.14
C2-H2	183.0	0.16	160.2	0.12
C1-H1	195.2	0.27	158.2	0.12
C18-H18a	145.5	0.31	148.2	0.28
C18-H18b	156.0	0.24	130.5	0.39
C20-H20a	121.6	0.39	130.4	0.03
C20-H20b	128.0	3.17	138.2	0.07
C22-H22	156.0	0.36	158.8	0.01
C23-H23a	154.5	0.18	145.5	0.02
C23-H23b	94.2	0.35	136.8	0.05
C12-H12	109.4	1.64	149.4	0.11
C11-H11a	152.2	0.27	135.3	0.05
C11-H11b	97.3	1.99	125.6	0.14

[a]Experimental errors are calculated as standard deviation of 10 separately measured peak positions. Each peak position is measured after adding noise from different parts of the spectrum. All couplings were extracted manually from the spectrum.

Table S3. Experimental LR $^{n}J_{CH}$ couplings, total couplings ($^{n}T_{CH}$) and errors. The number in brackets in the $^{n}J_{CH}$ coupling column is the n value.

Spin-pair	$\lvert {}^{n}T_{CH} \rvert = \lvert {}^{n}J_{CH} + {}^{n}D_{CH} \rvert$ (Hz)	error	$^{n}J_{CH}$ (Hz) (n)	error
C16-H15a	6.34	0.050	-1.74 (2)	0.450
C15-H1	6.81	0.041	3.46 (3)	0.170
C14-H16	6.92	0.041	6.48 (3)	0.017
C14-H22	8.61	0.027	8.83 (3)	0.014
C14-H15b	8.89	0.053	7.98 (3)	0.017
C13-H15a	4.46	0.100	3.56 (3)	0.050
C8-H16	7.72	0.050	6.95 (3)	0.020
C8-H12	5.68	0.046	5.84 (3)	0.029
C5-H8	3.45	0.022	3.32 (3)	0.018
C2-H4	8.89	0.018	7.62 (3)	0.012
C6-H4	6.64	0.060	5.62 (3)	0.030
C6-H16	3.66	0.043	2.27 (3)	0.015
C6-H8	4.24	0.056	3.76 (3)	0.016
C7-H15b	6.53	0.026	7.48 (3)	0.016
C7-H8	2.36	0.030	-1.16 (2)	0.400
C17-H8	7.99	0.310	5.91 (3)	0.030
C18-H20a	8.32	0.071	9.46 (3)	0.014
C10-H12	2.71	0.052	3.05 (3)	0.032
C20-H18b	4.57	0.063	7.57 (3)	0.010
C20-H22	7.26	0.036	5.94 (3)	0.011
C22-H20a	6.59	0.060	5.47 (3)	0.040
C23-H22	9.37	0.042	7.04 (2)	0.011
C12-H8	3.73	0.190	5.67 (3)	0.047

Table S4. Quality factors (Q) obtained from the alignment tensor optimization of the RDC and $^{n}T_{CH}$ data to each of the possible DFT-optimized configurations of strychnine.

Isomers	All RDCs	Long range RDCs	One-bond RDCs
RRRRRR	0.545164953	0.521748372	0.513023106
RRRRRS	0.652808190	0.525637182	0.638490245
RRRSRR	0.619690106	0.577686329	0.585120596
RRRSRS	0.240695577	0.543489870	0.195879637
RRSRRS	0.516550040	0.627347441	0.325411618
SRRRRR	0.423281739	0.492884180	0.410856896
SRRRRS	0.714410233	0.550610184	0.671000979
SRRSRR	0.553535910	0.223503243	0.554978002
SRRSRS	0.090509427	0.170545452	0.086892542
SRSRRR	0.809033392	0.609592355	0.825651680
SRSRRS	0.307511407	0.618501442	0.280106782
SRSSRR	0.881664450	0.456460962	0.878310482
SSRRRR	0.601344013	0.556087990	0.576791361
SSRRRS	0.615536795	0.524273679	0.593086975
SSRSRR	0.461354787	0.342261867	0.480565433
SSRSRS	0.185670256	0.209682925	0.189186016
SSSRRS	0.425979936	0.643699364	0.408958339
SSSSRS	0.614208001	0.564729072	0.623904117

Alignment tensor optimization and the relax analysis script:

Optimization of the experimental data for determining the alignment tensor was implemented in the software relax. Instead of using RDC values for the optimization as is usually the case, due to the nature of the signless *T* data, the *T* values were used instead. Non-linear least squares fitting of the alignment tensor using the Nelder-Mead Simplex algorithm was implemented by the construction of the following target function:

- The target function accepts the 5 unique alignment tensor parameters as input arguments.
- The alignment tensor matrix A is created from the 5 alignment tensor parameters.
- Using the matrix A, the signed RDC value for each bond vector is calculated.
- The signed J value is added to the signed RDC value to obtain a signed *T* value ($T = J+D$).
- The absolute value of this back-calculated *T* value is compared to the measured absolute *T* value using the standard chi-squared (χ^2) statistic.
- The target function returns the chi-squared value as required by optimization algorithms.

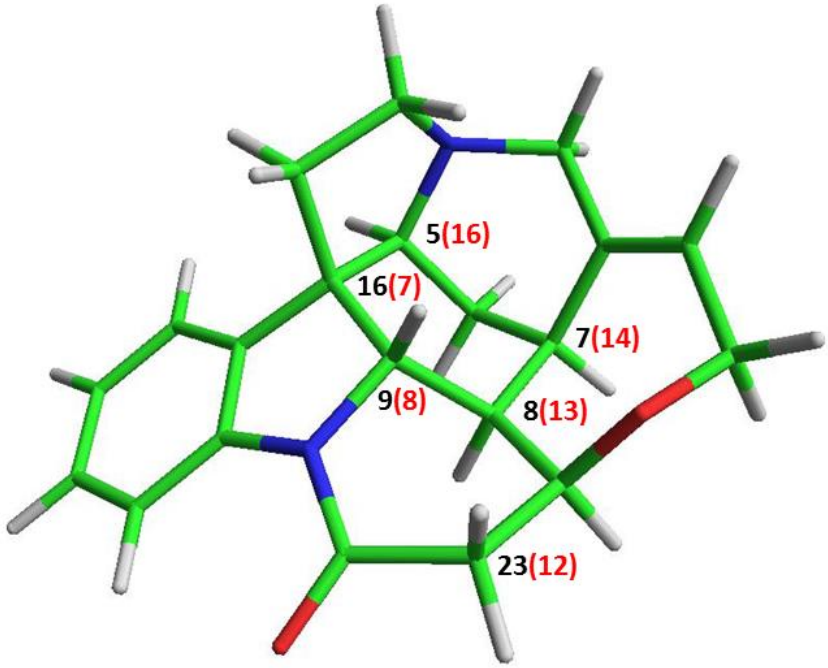
For comparison, the protocol for alignment tensor optimization using one-bond RDC data is:

- The target function accepts the 5 unique alignment tensor parameters as input arguments.
- The alignment tensor matrix A is created from the 5 alignment tensor parameters.
- Using the matrix A, the signed RDC value for each bond vector is calculated.
- This back-calculated *D* value is compared to the measured *D* value using the standard chi-squared (χ^2) statistic.
- The target function returns the chi-squared value as required by optimization algorithms.

The relax script used in the combined analysis for long range and one-bond RDC values is given below. For the long range only or one-bond only RDC analyses, the corresponding data loading functions were simply deleted in this script.

```
# Create the data pipe.
pipe.create('RRRRRR', 'N-state')

# Load the structure.
structure.read_gaussian(file='strychnine.log')

# Set up the 13C and 1H spins.
structure.load_spins(spin_id='@C*', ave_pos=False)
structure.load_spins(spin_id='@H*', ave_pos=False)

# Define the nuclear isotopes of all spins.
spin.isotope(isotope='13C', spin_id='@C*')
spin.isotope(isotope='1H', spin_id='@H*')

# Define the magnetic dipole-dipole interaction.
interatom.read_dist(file='one_bond_RDC', unit='Angstrom', spin_id1_col=1,
spin_id2_col=2, data_col=8)
interatom.read_dist(file='long_range_RDC', unit='Angstrom', spin_id1_col=1,
spin_id2_col=2, data_col=8)
interatom.unit_vectors(ave=False)

# Load the short range 1J signed RDCs.
rdc.read(align_id='gel', file='one_bond_RDC', data_type='T', spin_id1_col=1,
spin_id2_col=2, data_col=3, error_col=4, absolute=False)
j_coupling.read(file='one_bond_RDC', spin_id1_col=1, spin_id2_col=2,
data_col=5, error_col=6, sign_col=7)

# Load the long range J and J+D data.
rdc.read(align_id='gel', file='long_range_RDC', data_type='T',
spin_id1_col=1, spin_id2_col=2, data_col=3, error_col=4, absolute=True)
j_coupling.read(file='long_range_RDC', spin_id1_col=1, spin_id2_col=2,
data_col=5, error_col=6, sign_col=7)

# Set up the model.
n_state_model.select_model(model='fixed')

# Minimisation.
minimise.grid_search(inc=11)
minimise.execute('simplex')

# Show the tensors.
align_tensor.display()

# Create a correlation plot.
rdc.corr_plot(force=True)

# Save the relax state.
state.save('tensor', force=True)
```

DFT optimized structures of the eighteen different configurations:



The above is a DFT optimized structure of *SRRSRS*. The molecular numberings 7, 8, 12, 13, 14 and 16 (numbers inside the brackets) correspond to DFT numbering as changed by the Gaussian software to 16, 9, 23, 8, 7 and 5, respectively. The different configurations are built on the basis of the DFT numbering. The configuration *SRRSRS* designates configurations at carbon sites 5, 7, 8, 9, 16 and 23, respectively. In the following, DFT geometries for each diastereomer are presented in XYZ 3D structure format.

RRRRRR

O	2.818275	2.260813	-0.149742
O	-1.800351	3.154093	-0.924819
N	-1.309852	1.321881	0.334517
N	1.116243	-2.758269	-0.424978
C	0.558423	-1.727520	0.452171
C	1.227077	-1.558533	1.816221
C	2.133565	-0.383174	1.386684
C	1.146438	0.839782	1.013897
C	-0.325840	0.369434	0.836953
C	-2.503083	0.534214	0.223697
C	-3.812667	0.978484	0.175760
C	-4.829368	0.020105	0.149591
C	-4.535143	-1.339417	0.171639
C	-3.207933	-1.780126	0.193574
C	-2.185278	-0.849096	0.223380
C	-0.675208	-0.946278	0.023772
C	-0.390456	-1.076541	-1.535431
C	0.400256	-2.417478	-1.705094
C	2.593896	-2.362611	-0.382859

C	2.881836	-0.905686	0.123031
C	3.690449	-0.067252	-0.532299
C	3.941533	1.340787	-0.044715
C	1.513960	1.693664	-0.199992
C	0.510405	2.851987	-0.308380
C	-0.974528	2.461072	-0.344531
H	1.081235	-0.931412	-0.058791
H	1.795140	-2.439626	2.113089
H	0.551412	-1.315577	2.634812
H	2.838827	-0.041205	2.150031
H	1.149819	1.502027	1.885589
H	-0.669655	0.122995	1.844785
H	-4.037466	2.035553	0.167226
H	-5.862128	0.346070	0.122066
H	-5.340693	-2.063836	0.164769
H	-2.985041	-2.840769	0.180039
H	-1.313413	-1.108412	-2.111065
H	0.184966	-0.227352	-1.903544
H	-0.303179	-3.227538	-1.904967
H	1.098662	-2.375153	-2.541880
H	3.033670	-2.503070	-1.370375
H	3.090684	-3.063325	0.291913
H	4.163562	-0.371532	-1.460659
H	4.254186	1.326310	1.004162
H	4.740249	1.806898	-0.620976
H	1.440001	1.088178	-1.107220
H	0.654793	3.529289	0.540078
H	0.696241	3.432051	-1.211777

RRRRRS

O	-2.040735	1.962865	0.919504
O	1.984734	3.136601	0.758866
N	1.338070	1.225041	-0.289229
N	-1.348959	-2.743426	0.213886
C	-0.721774	-1.690774	-0.592483
C	-1.385098	-1.384380	-1.942919
C	-2.222020	-0.176093	-1.425261
C	-1.108114	0.956921	-1.180320
C	0.306003	0.359383	-0.850138
C	2.459190	0.357404	-0.114064
C	3.794007	0.702947	0.020138
C	4.733463	-0.329035	0.085406
C	4.342716	-1.662882	0.020213
C	2.990459	-2.002353	-0.089441
C	2.043088	-0.996978	-0.162457
C	0.521402	-0.987497	-0.061621
C	0.118284	-1.128045	1.465999
C	-0.683304	-2.469163	1.539571
C	-2.803834	-2.283192	0.130242
C	-2.934519	-0.748781	-0.145113
C	-3.494073	0.017537	0.795228
C	-3.407667	1.517523	0.849208
C	-1.462175	2.205228	-0.358818
C	-0.228103	3.105884	-0.177680
C	1.128137	2.486588	0.167202
H	-1.213326	-0.896651	-0.049710
H	-1.998287	-2.209477	-2.300684
H	-0.702109	-1.117948	-2.747875
H	-2.954142	0.220446	-2.137091
H	-0.965098	1.365541	-2.186771
H	0.696640	0.085885	-1.834943
H	4.094073	1.739815	0.066630
H	5.783838	-0.081102	0.180181
H	5.090993	-2.445259	0.061755
H	2.688907	-3.043318	-0.111095
H	0.985780	-1.165730	2.122368
H	-0.494324	-0.277419	1.771272
H	0.008124	-3.293155	1.726242
H	-1.416088	-2.464155	2.347521
H	-3.315674	-2.535579	1.057878

H	-3.275913	-2.858055	-0.667920
H	-3.916803	-0.465678	1.671038
H	-3.900891	2.000377	-0.003199
H	-3.884370	1.885600	1.757676
H	-2.196227	2.780283	-0.939609
H	-0.068571	3.657392	-1.110549
H	-0.438709	3.849694	0.589978

RRRSRR

O	-2.726428	2.345168	-0.431376
O	1.928176	3.393155	0.421542
N	1.282411	1.208478	0.592581
N	-1.268472	-2.856119	0.113376
C	-0.504417	-1.703021	-0.377021
C	-0.775945	-1.245461	-1.793062
C	-1.736937	-0.124346	-1.381950
C	-0.821198	0.841194	-0.561847
C	0.146007	0.294273	0.570063
C	2.421660	0.471455	0.163188
C	3.695030	0.958918	-0.106981
C	4.659485	0.060964	-0.565211
C	4.363242	-1.287133	-0.745280
C	3.084568	-1.768456	-0.458503
C	2.106820	-0.898014	-0.002910
C	0.683882	-1.176401	0.430216
C	0.493842	-2.116400	1.668889
C	-0.942123	-2.713491	1.576792
C	-2.694238	-2.344906	-0.228349
C	-2.803685	-0.782350	-0.477626
C	-3.713331	0.013826	0.094678
C	-3.859181	1.533523	-0.034519
C	-1.524791	1.939012	0.218084
C	-0.458638	3.041718	0.417031
C	1.034012	2.563211	0.485797
H	-1.130431	-1.021478	0.175577
H	-1.232990	-2.016913	-2.412704
H	0.110421	-0.874295	-2.308956
H	-2.190562	0.436786	-2.203467
H	-0.184672	1.309282	-1.320036
H	-0.378299	0.348390	1.524860
H	3.921110	2.005515	0.031805
H	5.656186	0.425643	-0.783527
H	5.127558	-1.965746	-1.103791
H	2.856475	-2.819858	-0.593077
H	1.231541	-2.917081	1.583790
H	0.659916	-1.615379	2.624951
H	-1.015120	-3.675897	2.083024
H	-1.651534	-2.026893	2.055585
H	-3.379153	-2.649921	0.562580
H	-2.997706	-2.859329	-1.141135
H	-4.451293	-0.412580	0.770962
H	-4.639412	1.777636	-0.760315
H	-4.204816	1.898330	0.941370
H	-1.816642	1.562732	1.202570
H	-0.478320	3.715492	-0.443306
H	-0.648208	3.653775	1.301339

RRRSRS

O	-2.457613	2.152637	0.573253
O	2.152165	3.309524	0.187381
N	1.318363	1.200069	0.502883
N	-1.394614	-2.770979	0.118097
C	-0.605511	-1.638500	-0.365996
C	-0.804691	-1.238510	-1.815693
C	-1.745028	-0.068370	-1.490574
C	-0.761138	0.929955	-0.751378
C	0.091732	0.401220	0.493512
C	2.406913	0.362609	0.149524
C	3.719489	0.737350	-0.116951

C	4.624605	-0.260699	-0.478095
C	4.232014	-1.593541	-0.568179
C	2.914048	-1.957062	-0.286140
C	1.996713	-0.982393	0.074788
C	0.547002	-1.114756	0.473220
C	0.261141	-1.973925	1.752788
C	-1.165825	-2.575264	1.592827
C	-2.782964	-2.267977	-0.330898
C	-2.838469	-0.708147	-0.572805
C	-3.701729	0.082706	0.069777
C	-3.648375	1.592905	-0.021291
C	-1.329065	2.274945	-0.301091
C	-0.241182	3.073662	0.475498
C	1.199918	2.559502	0.362182
H	-1.241894	-0.919010	0.133047
H	-1.261954	-2.026612	-2.412850
H	0.111576	-0.924352	-2.314929
H	-2.184740	0.444643	-2.353762
H	-0.022927	1.173420	-1.523462
H	-0.485087	0.583873	1.401899
H	4.017859	1.772365	-0.048572
H	5.651021	0.012363	-0.692617
H	4.951607	-2.351194	-0.853523
H	2.610206	-2.995962	-0.349928
H	0.999682	-2.777501	1.776299
H	0.358235	-1.410929	2.683043
H	-1.272383	-3.519056	2.127337
H	-1.903515	-1.872104	1.997767
H	-3.527109	-2.553416	0.411919
H	-3.028651	-2.787122	-1.257869
H	-4.420314	-0.343745	0.763345
H	-3.730461	1.940083	-1.057845
H	-4.475594	2.029756	0.537710
H	-1.640212	2.847660	-1.182868
H	-0.229598	4.120203	0.179388
H	-0.515988	3.041467	1.534394

RRSRRS

O	-2.741311	2.285863	0.399151
O	1.914692	3.337540	0.628639
N	1.301256	1.262960	-0.070745
N	-1.189619	-2.882526	0.237327
C	-0.564906	-1.781859	-0.528434
C	-1.222087	-1.399438	-1.850904
C	-2.087715	-0.270597	-1.255304
C	-1.148349	0.716617	-0.403427
C	0.301537	0.370815	-0.607377
C	2.499487	0.487142	-0.078882
C	3.809902	0.934562	-0.020165
C	4.831408	-0.013441	-0.116198
C	4.546269	-1.366975	-0.263699
C	3.221496	-1.813614	-0.295638
C	2.189428	-0.896481	-0.209257
C	0.683930	-1.050076	-0.003882
C	0.378109	-1.359225	1.523576
C	-0.470694	-2.682324	1.549090
C	-2.672805	-2.427102	0.224227
C	-2.957634	-0.924724	-0.159781
C	-3.753528	-0.072317	0.497765
C	-3.869555	1.410855	0.103435
C	-1.539414	2.169803	-0.409151
C	-0.439947	3.014827	0.276318
C	1.041543	2.555522	0.269638
H	-1.071029	-1.073091	0.084651
H	-1.830524	-2.203193	-2.265558
H	-0.536632	-1.080504	-2.633769
H	-2.685582	0.279240	-1.987170
H	-1.332759	0.488608	0.648064
H	0.522233	0.284012	-1.676457
H	4.025053	1.987699	0.087871

H	5.862433	0.317752	-0.083595
H	5.356042	-2.081698	-0.347464
H	3.005026	-2.872108	-0.383423
H	1.294182	-1.493580	2.095898
H	-0.164268	-0.528802	1.982731
H	0.201433	-3.533104	1.671655
H	-1.173998	-2.695070	2.382653
H	-3.113996	-2.648507	1.196118
H	-3.173801	-3.062843	-0.508427
H	-4.326645	-0.389741	1.363741
H	-4.122357	1.505588	-0.957866
H	-4.681350	1.861430	0.671938
H	-1.745701	2.552704	-1.414841
H	-0.437167	4.036141	-0.104216
H	-0.697948	3.086964	1.337363

SRRRRR

O	-2.822853	2.216834	0.065557
O	1.783080	3.173633	0.794985
N	1.289319	1.276258	-0.359164
N	-1.182702	-2.425668	0.739489
C	-0.252296	-2.146749	-0.406773
C	-1.074401	-1.760334	-1.649096
C	-1.980950	-0.554565	-1.306202
C	-1.125161	0.735347	-0.994223
C	0.310787	0.286852	-0.814495
C	2.494817	0.521169	-0.230896
C	3.804487	0.968347	-0.226504
C	4.818821	0.008299	-0.173426
C	4.520704	-1.350164	-0.126089
C	3.192152	-1.787639	-0.101773
C	2.175754	-0.851872	-0.156889
C	0.661011	-0.963345	0.040790
C	0.468975	-0.900247	1.586432
C	-0.841413	-1.599757	1.912199
C	-2.618197	-2.306042	0.417143
C	-2.906612	-0.943396	-0.162803
C	-3.783869	-0.068526	0.333276
C	-3.917425	1.318062	-0.239161
C	-1.525125	1.635962	0.175469
C	-0.533795	2.807070	0.247627
C	0.953108	2.441982	0.269185
H	0.338835	-3.044332	-0.612093
H	-1.690622	-2.603363	-1.964117
H	-0.420577	-1.546725	-2.495315
H	-2.598658	-0.327398	-2.179311
H	-1.153114	1.365213	-1.889482
H	0.653183	0.012876	-1.815127
H	4.030977	2.024151	-0.269089
H	5.852999	0.330885	-0.178744
H	5.324575	-2.075945	-0.099633
H	2.967612	-2.845896	-0.030561
H	1.300839	-1.438993	2.040954
H	0.513430	0.117338	1.975560
H	-0.746000	-2.225307	2.804475
H	-1.633955	-0.872712	2.117738
H	-3.189453	-2.476424	1.330517
H	-2.903488	-3.099728	-0.277945
H	-4.406246	-0.336589	1.181368
H	-4.018186	1.265490	-1.329996
H	-4.803729	1.818085	0.149613
H	-1.475613	1.070144	1.109759
H	-0.700672	3.460258	-0.615337
H	-0.718512	3.408390	1.137417

SRRRRS

O	1.927569	2.000297	-0.934699
O	-1.937771	3.215968	-0.582420
N	-1.263116	1.239813	0.315294

N	1.288652	-2.699569	-0.220558
C	0.451821	-2.064902	0.842973
C	1.372243	-1.448216	1.912693
C	2.143939	-0.255360	1.282622
C	1.142417	0.939228	1.201708
C	-0.252496	0.369340	0.929855
C	-2.375014	0.387300	0.075462
C	-3.704935	0.719841	-0.121676
C	-4.623502	-0.326259	-0.253282
C	-4.215828	-1.654294	-0.188688
C	-2.864444	-1.975861	-0.013275
C	-1.941575	-0.955319	0.117456
C	-0.414436	-0.946963	0.147269
C	0.050676	-0.964685	-1.342732
C	0.617943	-2.380756	-1.490827
C	2.701164	-2.245248	-0.191677
C	2.808030	-0.747172	-0.006025
C	3.357577	0.017972	-0.949193
C	3.274944	1.517268	-1.027077
C	1.487375	2.203563	0.401452
C	0.272262	3.139229	0.364880
C	-1.075309	2.538989	-0.029917
H	-0.192629	-2.826544	1.289953
H	2.060091	-2.207574	2.283868
H	0.796848	-1.119192	2.779218
H	2.949965	0.043057	1.962126
H	1.092681	1.317524	2.229002
H	-0.665170	0.131287	1.916543
H	-4.016791	1.753082	-0.166174
H	-5.671434	-0.092769	-0.398755
H	-4.948212	-2.447283	-0.280868
H	-2.551540	-3.013381	0.012445
H	-0.777847	-0.778839	-2.025679
H	0.811674	-0.213198	-1.529918
H	-0.196352	-3.096464	-1.645346
H	1.308210	-2.489054	-2.327955
H	3.172475	-2.554415	-1.124207
H	3.218298	-2.777812	0.610799
H	3.812107	-0.475234	-1.804099
H	3.885992	2.009572	-0.257817
H	3.640513	1.854411	-1.997363
H	2.293208	2.724269	0.937139
H	0.138172	3.577353	1.359720
H	0.465492	3.963206	-0.320836

SRRSRR

O	-2.778494	2.248529	-0.570474
O	1.780311	3.382672	0.528040
N	1.167369	1.187275	0.585031
N	-1.222348	-2.650004	0.343066
C	-0.171709	-2.114144	-0.573620
C	-0.810179	-1.435430	-1.778363
C	-1.734304	-0.314527	-1.291679
C	-0.865248	0.730085	-0.603848
C	0.059128	0.209386	0.494735
C	2.361960	0.544644	0.172112
C	3.623152	1.100152	-0.015118
C	4.639080	0.270622	-0.491891
C	4.405754	-1.074124	-0.764457
C	3.139340	-1.623013	-0.552234
C	2.115457	-0.815415	-0.083763
C	0.704956	-1.181761	0.318637
C	0.649044	-1.965667	1.653359
C	-0.811655	-2.412861	1.738226
C	-2.619352	-2.281603	0.032693
C	-2.795924	-0.822653	-0.342692
C	-3.736145	-0.005877	0.137977
C	-3.927783	1.475683	-0.156144
C	-1.598116	1.858086	0.118252
C	-0.576925	2.987253	0.312256

C	0.896281	2.537946	0.500274
H	0.460606	-2.942255	-0.913049
H	-1.358523	-2.170650	-2.371706
H	-0.031944	-1.026152	-2.427949
H	-2.212670	0.166166	-2.148528
H	-0.239589	1.166156	-1.390961
H	-0.482500	0.218117	1.441037
H	3.801083	2.142924	0.197401
H	5.626849	0.687010	-0.650153
H	5.209762	-1.699128	-1.133518
H	2.963376	-2.674246	-0.750302
H	1.316780	-2.827964	1.590223
H	0.959157	-1.364230	2.509519
H	-0.928080	-3.316452	2.343321
H	-1.426252	-1.632346	2.207172
H	-3.237178	-2.548836	0.891062
H	-2.963862	-2.905634	-0.799613
H	-4.468774	-0.399911	0.839166
H	-4.664139	1.617488	-0.952596
H	-4.340610	1.939828	0.748797
H	-1.904492	1.503059	1.105934
H	-0.553943	3.611355	-0.585555
H	-0.835628	3.644502	1.144805

SRRSRS

O	-2.547545	2.139059	0.472310
O	2.015408	3.324289	0.213156
N	1.207610	1.203922	0.478894
N	-1.350394	-2.624460	0.301178
C	-0.258837	-2.073956	-0.558021
C	-0.824223	-1.406962	-1.808433
C	-1.741283	-0.250780	-1.378644
C	-0.819735	0.828965	-0.783392
C	0.003153	0.334416	0.415455
C	2.358372	0.448322	0.162421
C	3.667689	0.888405	-0.010558
C	4.632616	-0.056196	-0.360560
C	4.303015	-1.398582	-0.525823
C	2.988069	-1.825141	-0.331972
C	2.015427	-0.899636	0.012625
C	0.561728	-1.122705	0.360284
C	0.390886	-1.834862	1.723978
C	-1.067936	-2.282629	1.709808
C	-2.708975	-2.252045	-0.131301
C	-2.815469	-0.775379	-0.431910
C	-3.718174	0.023460	0.134879
C	-3.726395	1.516213	-0.058936
C	-1.423939	2.193179	-0.407936
C	-0.372897	3.059448	0.332496
C	1.064718	2.558120	0.325331
H	0.399932	-2.896344	-0.855386
H	-1.364146	-2.140645	-2.409934
H	-0.007016	-1.035292	-2.430851
H	-2.229948	0.177326	-2.261725
H	-0.101863	1.055799	-1.581061
H	-0.582210	0.470722	1.326014
H	3.918694	1.929549	0.116264
H	5.656588	0.267474	-0.505165
H	5.068478	-2.115052	-0.797816
H	2.736463	-2.873299	-0.445917
H	1.059165	-2.698455	1.760657
H	0.631843	-1.189746	2.570301
H	-1.243126	-3.142405	2.361743
H	-1.719677	-1.470258	2.058429
H	-3.410692	-2.541912	0.651788
H	-2.971493	-2.840572	-1.016009
H	-4.455619	-0.395106	0.813636
H	-3.834304	1.785629	-1.118252
H	-4.559845	1.966160	0.480526
H	-1.736135	2.699031	-1.329897

H	-0.354638	4.078330	-0.048526
H	-0.690723	3.116119	1.378208

SRSRRR

O	-2.835216	2.183089	-0.366821
O	1.793058	3.420985	0.449377
N	1.267501	1.206350	0.221683
N	-1.256063	-2.564593	0.310645
C	-0.268677	-2.093906	-0.715873
C	-1.069094	-1.350176	-1.788433
C	-1.925986	-0.266978	-1.087687
C	-1.131616	0.493789	0.012250
C	0.288953	0.298665	-0.340109
C	2.498281	0.498299	0.087706
C	3.791719	0.993088	0.140691
C	4.842078	0.101877	-0.092140
C	4.600701	-1.241440	-0.361507
C	3.292564	-1.736360	-0.388176
C	2.233118	-0.874125	-0.170784
C	0.734296	-1.115451	0.034728
C	0.546392	-1.524101	1.528053
C	-0.814455	-2.219400	1.668075
C	-2.707518	-2.341607	0.045403
C	-3.030249	-0.883355	-0.274352
C	-3.908097	-0.068618	0.313913
C	-3.939201	1.463427	0.231617
C	-1.566943	1.940975	0.249964
C	-0.472911	2.900270	-0.251502
C	0.975914	2.548996	0.191771
H	0.266966	-2.950537	-1.136706
H	-1.723573	-2.045496	-2.317372
H	-0.416041	-0.928008	-2.552242
H	-2.307635	0.435086	-1.826538
H	-1.304073	-0.010029	0.954641
H	0.412989	0.388077	-1.424751
H	3.972201	2.038964	0.343730
H	5.860927	0.469496	-0.066521
H	5.431883	-1.911528	-0.544781
H	3.113427	-2.788903	-0.576301
H	1.348683	-2.218946	1.779191
H	0.648886	-0.670355	2.200543
H	-0.726391	-3.117630	2.288834
H	-1.545177	-1.571038	2.164713
H	-3.256234	-2.688832	0.921300
H	-3.008266	-2.988016	-0.783342
H	-4.640308	-0.463818	1.015060
H	-4.811641	1.798518	-0.335164
H	-4.068801	1.831387	1.259402
H	-1.681795	2.103163	1.328938
H	-0.466158	2.895665	-1.348543
H	-0.658291	3.924690	0.067515

SRSRRS

O	-2.817646	2.210078	0.226426
O	1.840113	3.350785	0.532999
N	1.275922	1.221818	-0.034713
N	-1.231701	-2.501558	0.571492
C	-0.264772	-2.164484	-0.529466
C	-1.072763	-1.599863	-1.702377
C	-1.947191	-0.445033	-1.166095
C	-1.139275	0.564911	-0.288932
C	0.291604	0.282518	-0.538956
C	2.499500	0.496695	-0.076749
C	3.799524	0.976182	-0.067233
C	4.837090	0.047320	-0.183282
C	4.575910	-1.314134	-0.299428
C	3.260193	-1.789898	-0.280745
C	2.215908	-0.890254	-0.174918

C	0.713311	-1.074253	0.053273
C	0.530472	-1.231913	1.593084
C	-0.835887	-1.868386	1.838021
C	-2.679823	-2.354585	0.271791
C	-3.010710	-0.960469	-0.231985
C	-3.898374	-0.082397	0.245176
C	-3.922350	1.374298	-0.214984
C	-1.547565	2.012889	-0.424786
C	-0.513542	2.908436	0.286107
C	0.983600	2.521334	0.247280
H	0.281427	-3.065580	-0.824016
H	-1.711635	-2.374329	-2.130734
H	-0.419583	-1.278898	-2.513909
H	-2.390610	0.088326	-2.010709
H	-1.334208	0.349428	0.760369
H	0.474513	0.226800	-1.617656
H	3.994610	2.035158	0.019306
H	5.861640	0.399533	-0.189512
H	5.397740	-2.013102	-0.397105
H	3.065748	-2.854620	-0.342098
H	1.321596	-1.893892	1.947779
H	0.651715	-0.284970	2.121588
H	-0.785180	-2.610787	2.640993
H	-1.573031	-1.120098	2.151314
H	-3.233559	-2.592982	1.180703
H	-2.963511	-3.106244	-0.469757
H	-4.601891	-0.367343	1.021714
H	-3.994030	1.434680	-1.307700
H	-4.798820	1.871642	0.197356
H	-1.635427	2.304007	-1.480121
H	-0.573949	3.936860	-0.069333
H	-0.772008	2.934195	1.349895

SRSSRR

O	-3.187588	1.814130	0.805009
O	1.300377	3.373424	-0.415643
N	1.040609	1.249554	0.351707
N	-0.958139	-2.607149	-0.273455
C	0.145640	-1.759073	-0.786218
C	-0.391945	-0.667835	-1.685589
C	-1.531199	0.008115	-0.930557
C	-1.230125	0.333408	0.566578
C	0.211600	0.181725	0.943070
C	2.321759	0.705933	0.089726
C	3.501802	1.368158	-0.228128
C	4.647578	0.597993	-0.432125
C	4.613210	-0.789164	-0.324334
C	3.417798	-1.440619	-0.012862
C	2.269703	-0.694378	0.197450
C	0.855152	-1.160364	0.477018
C	0.633399	-2.303056	1.483377
C	-0.781050	-2.829723	1.169493
C	-2.324406	-2.364577	-0.791313
C	-2.725446	-0.892398	-0.789669
C	-3.867801	-0.303501	-0.429019
C	-3.935624	1.215226	-0.291827
C	-1.755271	1.703496	0.939070
C	-0.936417	2.778229	0.205669
C	0.571463	2.496097	0.035623
H	0.880365	-2.376601	-1.316446
H	-0.766980	-1.078264	-2.626759
H	0.401329	0.033253	-1.948613
H	-1.807176	0.916935	-1.461702
H	-1.767975	-0.376291	1.189132
H	0.314464	0.244122	2.033391
H	3.522238	2.443556	-0.311317
H	5.579531	1.094680	-0.674504
H	5.516111	-1.366337	-0.482307
H	3.393325	-2.521697	0.062864
H	1.369394	-3.089994	1.304110

H	0.737572	-1.984151	2.521647
H	-0.872993	-3.890971	1.420276
H	-1.536357	-2.300193	1.765579
H	-3.022319	-2.966118	-0.207362
H	-2.374484	-2.747956	-1.816473
H	-4.749960	-0.875366	-0.158705
H	-3.657029	1.701322	-1.233242
H	-4.957545	1.517494	-0.067866
H	-1.313534	2.934323	-0.808554
H	-1.019072	3.743117	0.707742
H	-1.607429	1.845712	2.013823

SSRRRR

O	-2.860861	2.287787	0.166567
O	1.781367	3.222700	0.844275
N	1.270620	1.333540	-0.313071
N	-1.140167	-2.680639	0.443725
C	-0.248524	-2.191870	-0.677220
C	-1.197512	-1.597154	-1.706610
C	-1.815782	-0.500852	-0.814769
C	-1.178308	0.865470	-0.968325
C	0.299872	0.401826	-0.878640
C	2.465577	0.562808	-0.188018
C	3.772873	1.007613	-0.099942
C	4.788568	0.047621	-0.062194
C	4.494066	-1.310361	-0.113489
C	3.166681	-1.749013	-0.178318
C	2.147189	-0.815407	-0.215741
C	0.632130	-0.960995	-0.099690
C	0.314556	-1.004970	1.447664
C	-0.427488	-2.337628	1.679320
C	-2.624235	-2.367601	0.406164
C	-3.004109	-0.921397	-0.051224
C	-3.900566	-0.036983	0.392939
C	-3.920526	1.357140	-0.214837
C	-1.521603	1.789361	0.193689
C	-0.527071	2.953827	0.195866
C	0.947380	2.522332	0.283182
H	0.382766	-3.012751	-1.026039
H	-1.927037	-2.325266	-2.060167
H	-0.691537	-1.204313	-2.587177
H	-1.285717	-0.666457	0.109789
H	-1.351238	1.381859	-1.917748
H	0.637295	0.211413	-1.900583
H	3.995847	2.064220	-0.067159
H	5.820376	0.372141	-0.001919
H	5.298010	-2.036290	-0.096405
H	2.945111	-2.809912	-0.189421
H	1.230737	-0.958312	2.035078
H	-0.295642	-0.162170	1.769201
H	0.302988	-3.125393	1.892551
H	-1.110813	-2.295119	2.528021
H	-3.015630	-2.581188	1.400175
H	-3.094158	-3.081771	-0.272929
H	-4.602014	-0.271875	1.186958
H	-3.910412	1.273550	-1.305508
H	-4.830208	1.885001	0.067837
H	-1.398880	1.240407	1.132724
H	-0.654707	3.545074	-0.717176
H	-0.701369	3.620350	1.039739

SSRRRS

O	-2.231950	1.878798	0.754994
O	1.847175	3.104371	0.848974
N	1.325114	1.277735	-0.397544
N	-1.276915	-2.623556	0.355355
C	-0.352641	-2.152029	-0.738896
C	-1.260445	-1.527459	-1.790717
C	-1.862598	-0.383887	-0.936811

C	-1.121817	0.922119	-1.252122
C	0.334697	0.385849	-1.004608
C	2.456379	0.443138	-0.149822
C	3.779272	0.813034	0.015213
C	4.726780	-0.203760	0.166210
C	4.350339	-1.542473	0.150960
C	3.005617	-1.902502	0.006728
C	2.054775	-0.909484	-0.144453
C	0.533172	-0.947635	-0.147609
C	0.082309	-0.867639	1.363450
C	-0.657141	-2.196503	1.618092
C	-2.742597	-2.307115	0.199749
C	-3.047594	-0.818132	-0.135205
C	-3.803188	-0.005218	0.605820
C	-3.619598	1.490628	0.558352
C	-1.531160	2.171357	-0.456159
C	-0.330138	3.083169	-0.155612
C	1.035643	2.481134	0.172552
H	0.268761	-2.981794	-1.085354
H	-2.003012	-2.229090	-2.166793
H	-0.715338	-1.162304	-2.659458
H	-1.341293	-0.504152	-0.005266
H	-1.184841	1.190101	-2.310482
H	0.742637	0.134503	-1.987148
H	4.067104	1.854397	0.022843
H	5.770368	0.060000	0.288528
H	5.103059	-2.314146	0.258595
H	2.717593	-2.947280	0.023985
H	0.940266	-0.759837	2.026217
H	-0.568540	-0.010537	1.554780
H	0.066528	-2.958575	1.926442
H	-1.402056	-2.118623	2.410729
H	-3.228736	-2.584440	1.134076
H	-3.143299	-2.966887	-0.570533
H	-4.421589	-0.412862	1.399323
H	-3.973300	1.931071	-0.380815
H	-4.172814	1.959463	1.372896
H	-2.218269	2.745588	-1.088351
H	-0.160299	3.715176	-1.034292
H	-0.582504	3.756068	0.662968

SSRSRR

O	-2.824872	2.437563	-0.177358
O	1.856920	3.437928	0.385520
N	1.279358	1.231046	0.479182
N	-1.297224	-2.695223	0.323498
C	-0.183003	-2.150232	-0.570449
C	-0.850910	-1.356487	-1.664322
C	-1.653444	-0.413974	-0.770090
C	-0.928970	0.863706	-0.504418
C	0.148280	0.321181	0.480395
C	2.429499	0.518733	0.071139
C	3.701003	1.018267	-0.183539
C	4.684171	0.123717	-0.606609
C	4.405535	-1.230783	-0.764262
C	3.126544	-1.721949	-0.493526
C	2.129670	-0.854142	-0.075304
C	0.698852	-1.163241	0.329788
C	0.560019	-1.929364	1.675214
C	-0.907398	-2.392938	1.724307
C	-2.746354	-2.360789	-0.018419
C	-3.003967	-0.845476	-0.406061
C	-3.953743	0.073616	-0.190883
C	-3.759785	1.473733	-0.784657
C	-1.606349	1.918365	0.342671
C	-0.517167	3.012683	0.537837
C	0.991269	2.578624	0.463798
H	0.445977	-2.978826	-0.905678
H	-1.471172	-1.971410	-2.317633
H	-0.130230	-0.829241	-2.291167

H	-1.403660	-0.796365	0.212591
H	-0.484680	1.313942	-1.396340
H	-0.321585	0.362201	1.465334
H	3.910159	2.070377	-0.058919
H	5.680649	0.495050	-0.814136
H	5.183994	-1.908467	-1.092601
H	2.919162	-2.779643	-0.608982
H	1.227565	-2.793917	1.653653
H	0.830674	-1.324867	2.542579
H	-1.028545	-3.270403	2.364657
H	-1.540678	-1.601701	2.151296
H	-3.348980	-2.668595	0.836077
H	-3.043959	-2.989160	-0.859042
H	-4.872146	-0.136797	0.347624
H	-3.451960	1.361270	-1.827796
H	-4.704896	2.014669	-0.772445
H	-1.845652	1.474368	1.314971
H	-0.618900	3.750115	-0.261675
H	-0.644971	3.553212	1.477915

SSRSRS

O	-2.577021	2.084912	0.452112
O	2.045156	3.379287	0.176912
N	1.308935	1.224338	0.413353
N	-1.419768	-2.611787	0.296193
C	-0.258434	-2.126277	-0.553885
C	-0.854655	-1.384617	-1.728987
C	-1.656836	-0.336703	-0.948391
C	-0.806611	0.914390	-0.789274
C	0.105023	0.402396	0.366576
C	2.430779	0.428182	0.101007
C	3.742252	0.838430	-0.109227
C	4.690245	-0.135891	-0.421018
C	4.337862	-1.479294	-0.513679
C	3.018143	-1.877152	-0.289684
C	2.056600	-0.926551	0.017353
C	0.590000	-1.120297	0.350571
C	0.336019	-1.788235	1.729492
C	-1.140493	-2.212852	1.697273
C	-2.814006	-2.277302	-0.183324
C	-3.019412	-0.762635	-0.545836
C	-3.951528	0.088504	-0.110036
C	-3.750540	1.582554	-0.253634
C	-1.405980	2.245056	-0.358354
C	-0.340734	3.035182	0.462264
C	1.126767	2.582534	0.320478
H	0.375668	-2.976236	-0.820602
H	-1.464351	-2.027819	-2.363944
H	-0.087849	-0.937241	-2.360878
H	-1.447607	-0.651035	0.067568
H	-0.205520	1.096945	-1.683537
H	-0.473124	0.558215	1.281962
H	4.007231	1.882474	-0.035947
H	5.717200	0.163670	-0.593034
H	5.089690	-2.220342	-0.755968
H	2.753297	-2.926272	-0.353620
H	0.979836	-2.666676	1.815097
H	0.560779	-1.129942	2.570292
H	-1.337318	-3.037885	2.386655
H	-1.783909	-1.377558	2.009744
H	-3.505578	-2.577274	0.603962
H	-3.029538	-2.902423	-1.050431
H	-4.800761	-0.260122	0.469247
H	-3.673965	1.880096	-1.305335
H	-4.593791	2.118495	0.182567
H	-1.682181	2.824048	-1.246704
H	-0.365833	4.096816	0.227236
H	-0.608381	2.932079	1.518557

SSSRRS

O	-2.823564	2.359372	0.240082
O	1.897305	3.416959	0.540772
N	1.286290	1.286081	0.026907
N	-1.212795	-2.799681	0.175108
C	-0.291901	-2.134217	-0.848324
C	-1.233939	-1.315978	-1.723262
C	-1.824452	-0.445502	-0.589855
C	-1.122748	0.805875	-0.152330
C	0.270210	0.411045	-0.504677
C	2.482541	0.519741	-0.020423
C	3.795634	0.958025	0.048764
C	4.811252	0.007374	-0.079286
C	4.516760	-1.338662	-0.268411
C	3.188455	-1.774788	-0.314404
C	2.161858	-0.855141	-0.193397
C	0.651421	-1.051211	-0.041965
C	0.337685	-1.398374	1.460824
C	-0.482034	-2.713003	1.449002
C	-2.713904	-2.460254	0.214391
C	-3.063965	-0.929387	-0.011667
C	-3.957242	-0.015665	0.393912
C	-3.888901	1.428272	-0.162832
C	-1.557085	2.197573	-0.444241
C	-0.465425	3.110972	0.172099
C	1.023277	2.612902	0.242541
H	0.306072	-2.898298	-1.349269
H	-1.991291	-1.943060	-2.193202
H	-0.743278	-0.769246	-2.524680
H	-1.340230	-0.929916	0.239606
H	-1.192857	0.797045	0.943822
H	0.401111	0.418689	-1.591406
H	4.016244	2.006516	0.187499
H	5.844487	0.330614	-0.038041
H	5.321116	-2.056348	-0.374894
H	2.967685	-2.828751	-0.439026
H	1.258080	-1.520048	2.030985
H	-0.220142	-0.596563	1.950443
H	0.204819	-3.563120	1.514854
H	-1.164570	-2.784098	2.296395
H	-3.082203	-2.827861	1.171372
H	-3.201790	-3.051807	-0.561295
H	-4.787916	-0.246116	1.054737
H	-3.879078	1.380336	-1.257338
H	-4.794659	1.953791	0.136986
H	-1.693321	2.407214	-1.512210
H	-0.419721	4.082838	-0.318858
H	-0.737943	3.305150	1.213822

SSSSRS

O	-2.928471	2.235165	0.255387
O	1.723052	3.420290	-0.170034
N	1.190421	1.285369	0.419363
N	-1.096643	-2.785812	-0.322406
C	-0.062880	-1.776888	-0.792597
C	-0.820326	-0.603836	-1.297824
C	-1.670390	-0.408149	-0.000324
C	-1.211187	0.745661	0.777821
C	0.264772	0.314859	1.017322
C	2.368853	0.598227	0.040789
C	3.594480	1.138612	-0.337676
C	4.625409	0.262837	-0.674259
C	4.438592	-1.115643	-0.636154
C	3.203883	-1.643511	-0.258561
C	2.163607	-0.793260	0.088329
C	0.740611	-1.164528	0.464008
C	0.553683	-2.331119	1.469119
C	-0.751599	-3.100057	1.094780
C	-2.578457	-2.454967	-0.578556
C	-2.976530	-0.920076	-0.340373

C	-3.992097	-0.079340	-0.540090
C	-3.840835	1.467878	-0.585806
C	-1.516400	2.022070	0.048856
C	-0.553458	3.086775	0.558119
C	0.893631	2.621149	0.247270
H	0.641465	-2.257597	-1.475501
H	-1.437634	-0.801800	-2.173721
H	-0.171400	0.235236	-1.540813
H	-1.372613	-1.161154	0.699342
H	-1.721778	0.809370	1.741585
H	0.465717	0.278845	2.092410
H	3.733433	2.207763	-0.365435
H	5.586850	0.668235	-0.966277
H	5.251972	-1.780922	-0.898988
H	3.061588	-2.718116	-0.238810
H	1.405586	-3.006533	1.373865
H	0.532870	-1.996790	2.508317
H	-0.604188	-4.175695	1.223849
H	-1.571559	-2.816666	1.764620
H	-3.151366	-3.123102	0.064040
H	-2.805501	-2.729292	-1.608593
H	-4.981588	-0.408126	-0.852277
H	-3.616721	1.729276	-1.630251
H	-4.809991	1.907054	-0.349429
H	-1.354736	1.917523	-1.029452
H	-0.668195	4.056265	0.076106
H	-0.665471	3.225533	1.638733

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