Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Extending Molecular Dynamics with Dipolar NMR Tensors as Constraints to Chiral Phosphorus Compounds

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1. Experimental Section

1.1. Instrumentation

For structural assignment, NMR spectra were recorded on a Bruker Avance III HD 500 spectrometer with a broad-band cryo-probe, with an ATM module (5 mm CPBBO BB-^{1}H/^{19}F/^{15}N/D Z-GRD), operating at 499.98 MHz for ^{1}H, at 125.73 MHz for ^{13}C and at 202.39 MHz for ^{31}P.

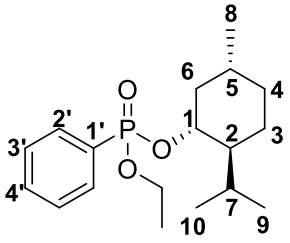
For RDC analysis, NMR spectra were recorded on a Bruker Avance III HD 600 spectrometer with an inverse triple resonance cryo-probe, with an ATM module (5 mm CPTCI ^{1}H/^{13}C/^{15}N/D Z-GRD), operating at 600.13 MHz for ^{1}H and at 150.92 MHz for ^{13}C.

HR-MS spectra were recorded on an LTQ Orbitrap XL (Thermo Fisher Scientific) using atmospheric-pressure chemical ionization (APCI).

1.2. Synthesis and diastereomer separation of 3

Starting compounds and solvents were purchased from Sigma Aldrich (EU) and directly used for synthesis. Gradient Flash chromatography was performed on Compact preparative system ECOM (CZ) using manually pre-filed silica (Silica gel 60, 0.040-0.063 mm, Merck) cartridges.

Ethyl ((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl) (*R*)-phenylphosphonate and ethyl ((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl) (*S*)-phenylphosphonate



Ethyl phenylphosphinate (94%, 620 µL, 5.2 mmol) was added to a mixture of L-menthol (630 mg, 4 mmol) and *N*-methylimidazole (500 mg, 6 mmol) in tetrachloromethane (10 mL). The reaction was stirred overnight and quenched by adding water (20 mL). The water phase was extracted with dichloromethane (3 x 15 mL), dried with magnesium sulfate, and evaporated. Gradient Flash chromatography on silica (Hexane/EtOAc, 0−100%) afforded the title products, 743 mg (44 %), a colorless solid.

The diastereomers of **3** (3A and 3B) were separated by semi-preparative HPLC with a chiral phase column under the following conditions: ChiralArt Cellulose-SB (250 x 20 mm, 5 µm, YMC), heptane, 0.1% IPA @20 mL/min, t_{R1} = 16:40 min, t_{R2} = 19.52 min. The HPLC instrument used to separate the diastereomers was a Puriflash PF5.250 chromatograph (Interchim) equipped with a diode array detector. The reproducibility of the separation was very limited.

3A dataset:

^{1}H NMR (500 MHz, $CDCl_3$, 25°C): δ = 7.81 (m, 2H, 2'), 7.53 (m, 1H, 4'), 7.45 (m, 2H, 3'), 4.21 (m, 1H, 1), 4.12 (m, 1H, -O-**CH_2**-CH_3), 4.04 (m, 1H, -O-**CH_2**-CH_3), 2.33 (dm, J_{Gem} = 12.0, 6a), 1.87 (m, 1H, 7), 1.67–1.58 (m, 2H, 3a, 4a), 1.52–1.41 (m, 1H, 5), 1.36–1.28 (m, 4H, -O-CH_2-**CH_3**, 2), 1.22 (dm, 1H, J_{Gem} = 12.0, 6b), 0.99–0.90 (m, 4H, 3b, 5-**CH_3**), 0.86 (dm, 1H, J_{Gem} = 12.8, 4b), 0.79 (d, 3H, $J_{10\text{-}7}$ = 7.1, 10), 0.47 (m, 3H, $J_{9\text{-}7}$ = 6.9, 9) ppm.

^{13}C NMR (125 MHz, $CDCl_3$, 25°C): δ = 132.25 (d, $J_{4'-P}$ = 3.1, 4'), 131.91 (d, $J_{2'-P}$ = 9.9, 2'), 129.16 (d, $J_{1'-P}$ = 188.4, 1'), 128.45 (d, $J_{3'-P}$ = 15.4, 3'), 77.85 (d, J_{1-P} = 6.5, 1), 61.97 (d, J_{CH2-P} = 5.4, -O-**CH_2**-CH_3), 48.66 (d, J_{2-P} = 6.9, 2), 43.51 (6), 34.24 (4), 31.72 (5), 25.63 (7), 22.88 (3), 22.16 (8), 21.06 (10), 16.46 (d, J_{CH3-P} = 6.7, -O-CH_2-**CH_3**), 15.36 (9) ppm.

^{31}P NMR (202 MHz, $CDCl_3$, 25°C): δ = 17.98 ppm.

HR-MS (APCI) calculated for $C_{18}H_{30}O_3P$, $[M+H]^+$ m/z: 325.19271, found $[M+H]^+$ 325.19282.

3B dataset:

^{1}H NMR (500 MHz, $CDCl_3$, 25°C): δ = 7.81 (m, 2H, 2'), 7.53 (m, 1H, 4'), 7.45 (m, 2H, 3'), 4.34 (m, 1H, 1), 4.12 (m, 1H, -O-**CH_2**-CH_3), 4.03 (m, 1H, -O-**CH_2**-CH_3), 2.23 (m, 1H, 7), 2.09 (dm, 1H, J_{Gem} = 12.2, 6a), 1.70–1.59 (m, 2H, 3a, 4a), 1.46–1.34 (m, 2H, 5, 2), 1.29 (t, 3H, $J_{CH3\text{-}CH2}$ = 7.1, -O-CH_2-**CH_3**), 1.09 (dm, 1H, J_{Gem} = 12.2, 6b), 1.02 (m, 1H, 3b), 0.93 (d, 3H, $J_{10\text{-}7}$ = 7.1, 10), 0.86–0.80 (m, 7H, 4b, 11, 8) ppm.

^{13}C NMR (125 MHz, $CDCl_3$, 25°C): δ = 132.25 (d, $J_{4'-P}$ = 3.1, 4'), 131.80 (d, $J_{2'-P}$ = 9.4, 2'), 129.92 (d, $J_{1'-P}$ = 189.4, 1'), 128.48 (d, $J_{3'-P}$ = 15.0, 3'), 78.13 (d, J_{1-P} = 7.0, 1), 62.09 (d, J_{CH2-P} = 5.2, -O-**CH_2**-CH_3), 48.75 (d, J_{2-P} = 6.2, 2), 43.18 (6), 34.21 (4), 31.66 (5), 25.72 (7), 22.97 (3), 22.05 (8), 21.18 (10), 16.46 (d, J_{CH3-P} = 6.9, -O-CH_2-**CH_3**), 15.79 (9) ppm.

^{31}P NMR (202 MHz, $CDCl_3$, 25°C): δ = 17.37 ppm.

HR-MS (APCI) calculated for $C_{18}H_{30}O_3P$, $[M+H]^+$ m/z: 325.19271, found $[M+H]^+$ 325.19278.

1.3. NMR and HR-MS spectra of 3

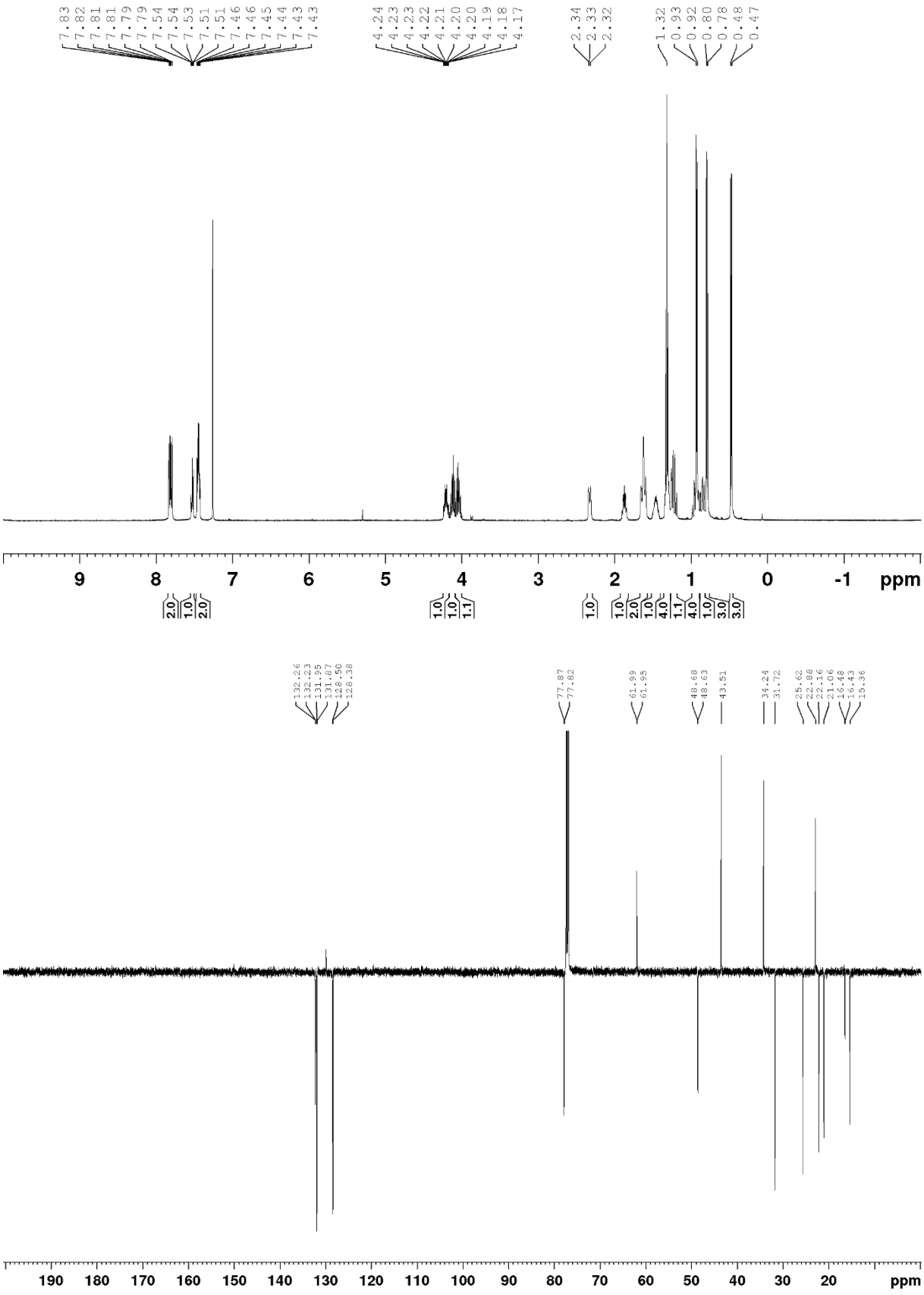


Figure S1: ^{1}H (top) and ^{13}C APT (bottom) NMR spectra of **3A** in $CDCl_3$ measured at room temperature

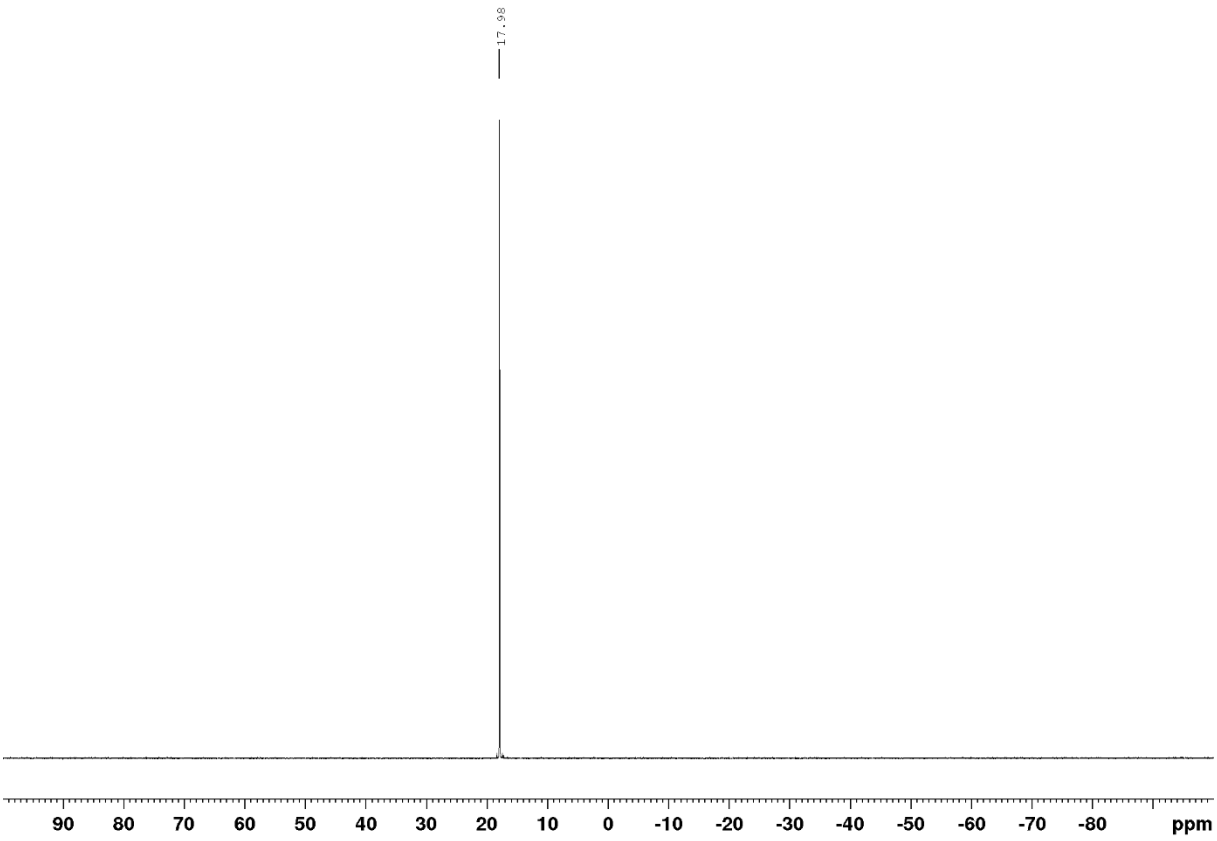


Figure S2: ^{31}P NMR spectrum of **3A** in $CDCl_3$ measured at room temperature

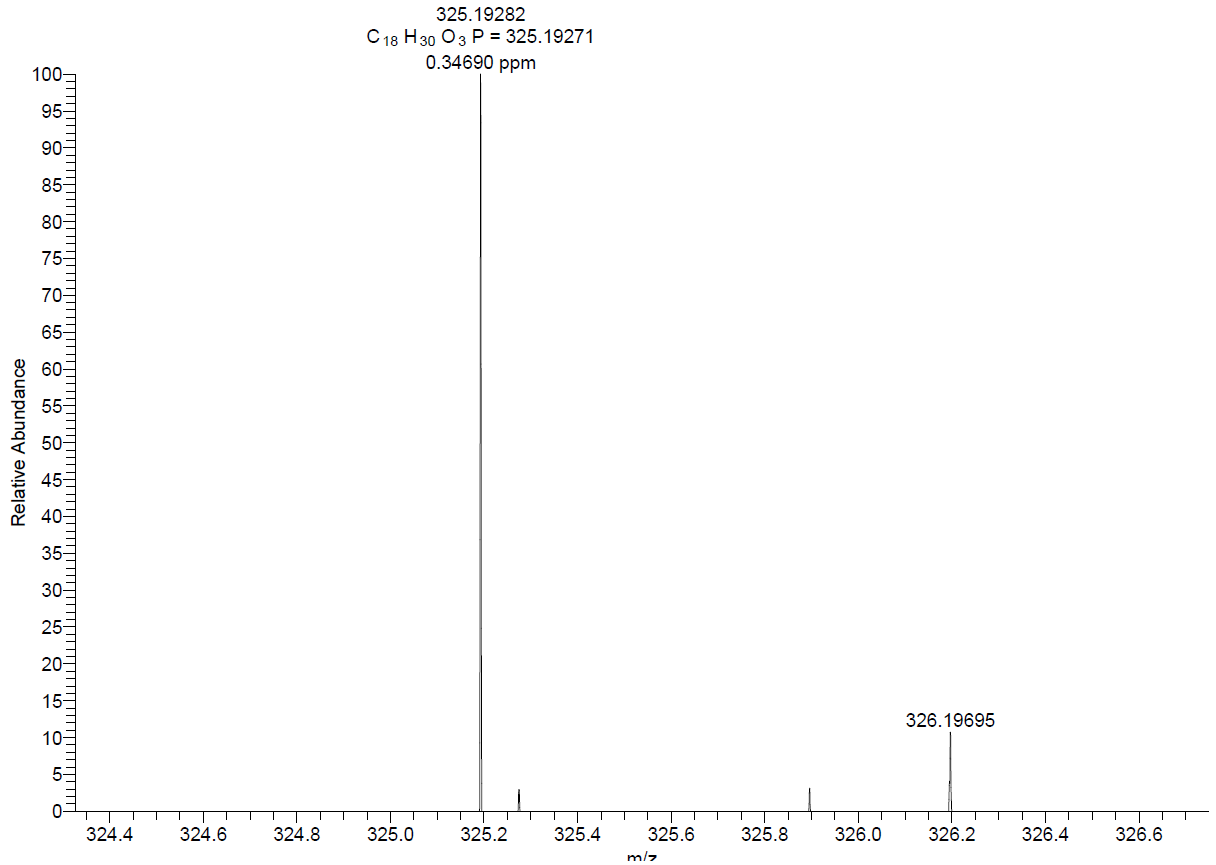


Figure S3: HR-MS spectrum of **3A**

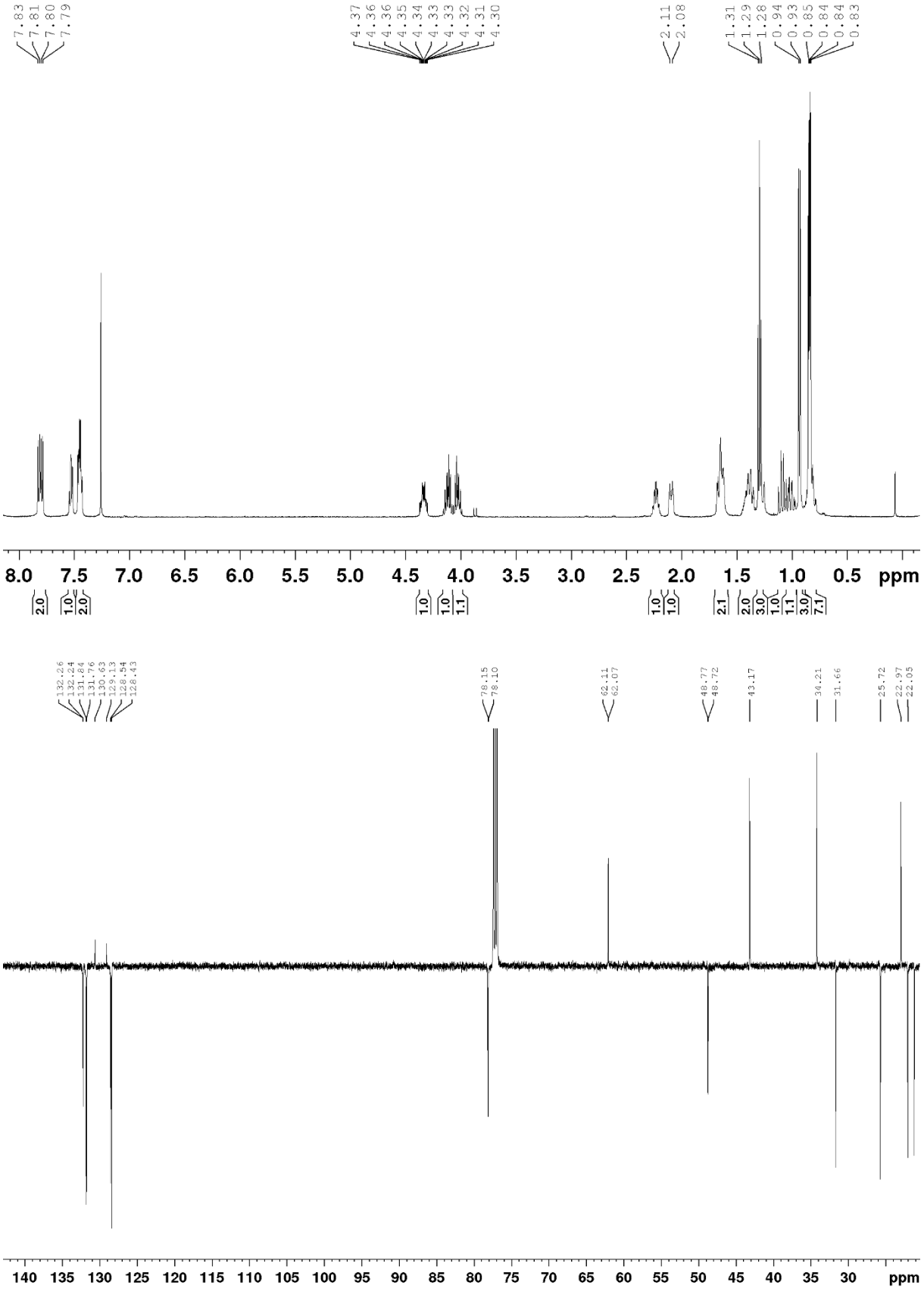


Figure S4: ^{1}H (top) and ^{13}C APT (bottom) NMR spectra of **3B** in $CDCl_3$ measured at room temperature

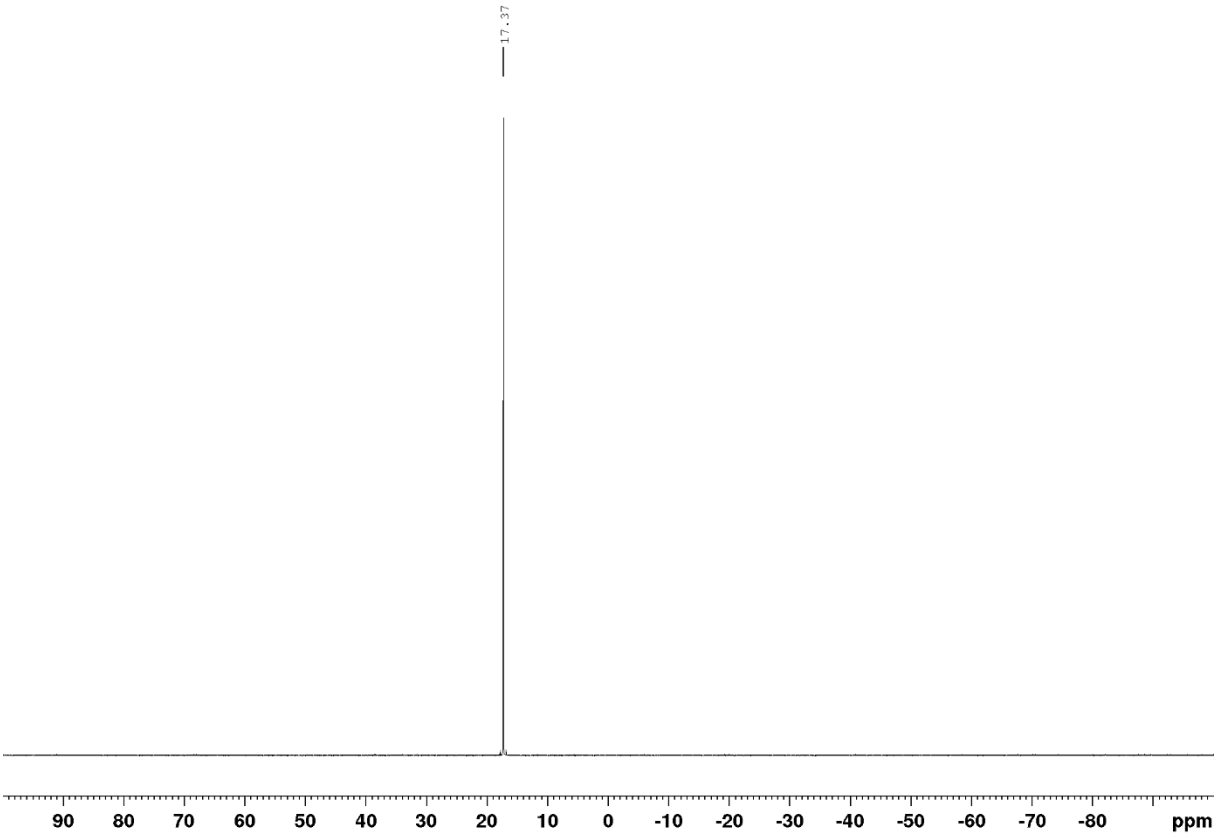


Figure S5: ^{31}P NMR spectrum of **3B** in $CDCl_3$ measured at room temperature

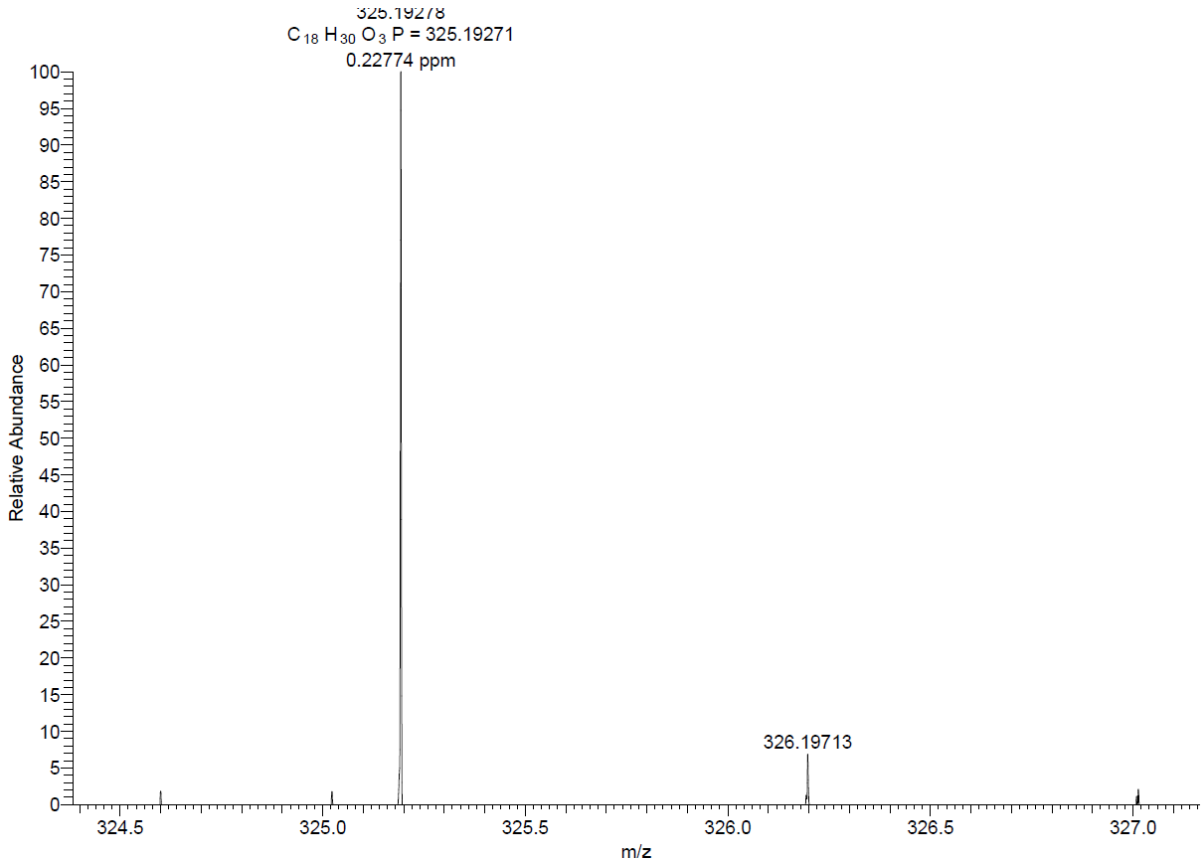


Figure S6: HR-MS spectrum of **3B**

1.4. Composition of the samples prepared for RDC analysis

Table S1: Composition of individual samples prepared for RDC measurements

Compound	m (compound) [mg]	m ($CDCl_3$) [mg]	m (PBLG) [mg]	w (medium) [%]
3A	4.9	900.0	68.3	7.0
3B	5.2	900.0	73.0	7.5

Sample preparation, RDC analysis and Boltzmann distribution were conducted as described in our previous studies.[1, 2] Poly-γ-benzyl-L-glutamate (PBLG) was used as an alignment medium.

1.5. Low-energy study of compound 3

Conformational sampling

Conformational sampling was performed using MacroModel v13.1 (Schrödinger 2022-1 suite)[3, 4] with the following set of parameters: OPLS4 force field,[5] chloroform solvent, mixed torsional/low-mode sampling method with a maximum of 1000 steps, 40 kJ/mol energy window for saving structures, and 0.75 Å maximum atom deviation cut-off.

Density functional theory (DFT) calculations

DFT calculations were performed using the Gaussian 16 program package.[6] Geometry optimizations of the conformers derived from conformational sampling were performed *in vacuo* using the B3LYP functional[7-10] with empirical dispersion correction (GD3)[11] and the 6-31+G(d,p) basis set.[12]

Machine learning-aided elimination of redundant structures

Unique conformers were identified using the machine learning (ML)-based mean-shift algorithm[13] as implemented in the Scikit-learn Python package (scikit-learn.org). During the ML-aided elimination procedure, the conformers were sorted into clusters based on dihedral angles. Each cluster contained all conformers with similar dihedral angles. The cluster size was specified by the mean shift clustering algorithm using a bandwidth parameter. The value of this parameter determines whether each data point belongs to a given cluster, i.e., whether a given set of conformers is similar enough. This parameter is approximately proportional to the size of a given cluster. The optimal value of isomers of

3 was 20. For each cluster, only the lowest energy conformer was selected as the unique non-redundant conformer.

Calculations of conformer populations

The relative populations of conformers were calculated using Boltzmann distribution according to equation S1:

$$p_i = \frac{e^{\frac{E_0 - E_i}{R \cdot T}}}{\sum_i e^{\frac{-E_i}{R \cdot T}}} \quad \text{(S1)}$$

Where p_i is the relative population of conformer i, E_0 is the energy of the global minimum, E_i is the energy of conformer i, R is the universal gas constant, and T is the thermodynamic temperature. The temperature 298.15 K (25 °C) was considered thoroughly. Of all the nonredundant conformers, only the conformers populated by more than 2% were used in further calculations of RDC parameters.

P3D/PALES

We performed molecular alignment simulations using P3D[14] as implemented in PALES[15] software and as recommended by the authors.[16] The following command was used to run the simulation:

pales -elPales -3D -pot3D PBLG.dx -lcS 0.8 -maxPot 2 -z1 150 -zN 250 -nX 129 -nY 129 -nZ 385 -dX 0.4 -dY 0.4 -dZ 0.4 -H -nosurf -pdb Molecule.pdb -inD RDCs.tbl -wv 0.12 -rM 8 -pka charges.pka -outD output.out,

where PBLG.dx is the potential file of PBLG, Molecule.pdb is the PDB file of the studied molecule, RDCs.tbl is the list of experimental RDCs, charges.pka is the list of atomic charges obtained from AtomicChargeCalculator II,[17] and output.out is the final output file. Atomic charges were calculated using the electronegativity equalization method (EEM)[18] based on the atoms in molecules (AIM) calculation scheme at the B3LYP/6-311G level of theory.[19]

Calculation of nConf20

We calculated the values of the flexibility descriptor $nConf_{20}$ using the code, as provided in the original article by Wicker and Cooper.[20] Because a more detailed scale was needed for these compounds, we set the atom root-mean-square (RMS) distance threshold to 0.5 Å to remove duplicate conformers. The number of generated conformers was set to 10,000 to alleviate stochasticity effects on the structure generation process.

Table S2: Theoretical (calculated) RDCs of the low-energy conformers of **3-RR** normalized against the 3A experimental dataset

Atoms	Experimental RDCs [Hz]	Theoretical Normalized RDCs [Hz]							
		Conformer							
		A	B	C	D	E	F	G	H
C4'-H4'	1.76	-13.24	-11.42	-10.00	-14.72	-18.97	-22.88	-14.33	-6.27
C1-H1	24.13	23.93	23.64	20.78	24.93	22.76	23.00	24.04	23.37
C2-H2	25.48	23.95	23.64	20.56	23.18	22.52	22.70	22.64	22.45
C5-H5	25.63	23.99	23.65	20.16	23.22	22.25	22.32	22.62	23.32
C7-H7	-5.17	-4.19	-5.25	-20.53	-4.30	-6.39	-3.86	-5.81	-10.18
CH_2-**C**H_3	-0.09	1.61	-0.71	-2.14	0.73	-2.52	-2.49	-2.96	-0.84
C5-C8	-0.58	-0.59	-0.65	0.05	-0.04	-0.22	-0.30	0.14	-1.01
C4'-P	-0.01	-0.07	-0.06	-0.05	-0.08	-0.10	-0.12	-0.07	-0.03
C1'-P	0.21	-1.17	-1.00	-0.77	-1.20	-1.66	-2.05	-1.12	-0.51
C1-P	0.55	-0.35	-0.36	-0.58	-0.74	-0.55	-0.48	-0.73	-0.39
C2-P	-0.21	-0.13	-0.12	-0.14	-0.14	-0.10	-0.07	-0.14	-0.09
R		0.935	0.953	0.919	0.924	0.896	0.857	0.932	0.979
Q		0.677	0.690	0.645	0.443	0.574	0.592	0.475	0.604

Table S3: Theoretical (calculated) RDCs of the low-energy conformers of **3-RR** normalized against 3B experimental dataset

Atoms	Experimental RDCs [Hz]	Theoretical Normalized RDCs [Hz]							
		Conformer							
		A	B	C	D	E	F	G	H
C4'-H4'	6.80	-16.54	-14.13	-11.87	-18.29	-23.65	-28.88	-17.68	-7.62
C1-H1	29.63	29.88	29.25	24.67	30.98	28.39	29.04	29.66	28.39
C2-H2	30.36	29.91	29.25	24.41	28.80	28.08	28.66	27.93	27.27
C5-H5	30.49	29.97	29.26	23.94	28.85	27.75	28.18	27.91	28.33
C7-H7	-7.72	-5.23	-6.49	-24.38	-5.35	-7.97	-4.88	-7.17	-12.37
CH_2-**C**H_3	-0.24	2.02	-0.88	-2.54	0.90	-3.15	-3.14	-3.66	-1.03
C4'-P	-0.07	-0.09	-0.08	-0.06	-0.09	-0.13	-0.16	-0.09	-0.04
C1'-P	0.76	-1.47	-1.24	-0.92	-1.50	-2.07	-2.59	-1.38	-0.62
C1-P	0.72	-0.44	-0.44	-0.69	-0.92	-0.69	-0.61	-0.90	-0.47
C2-P	-0.25	-0.16	-0.14	-0.16	-0.17	-0.12	-0.09	-0.18	-0.11
R		0.893	0.917	0.913	0.882	0.851	0.803	0.895	0.961
Q		0.687	0.701	0.655	0.445	0.588	0.608	0.479	0.604

Table S4: Boltzmann distribution-weight averaged RDCs of **3-RR** conformers normalized against the 3A experimental dataset

Atoms	Experimental RDCs [Hz]	Normalized Boltzmann averaged RDCs [Hz]
C4'-H4'	1.76	-11.30
C1-H1	24.13	20.90
C2-H2	25.48	20.74
C5-H5	25.63	20.69
C7-H7	-5.17	-7.08
CH_2-**C**H_3	-0.09	-0.22
C5-C8	-0.58	-0.39
C4'-P	-0.01	-0.06
C1'-P	0.21	-0.97
C1-P	0.55	-0.39
C2-P	-0.21	-0.11
R		0.946

Table S5: Boltzmann distribution-weight averaged RDCs of conformers of **3-RR** normalized against the 3B experimental dataset

Atoms	Experimental RDCs [Hz]	Normalized Boltzmann averaged RDCs [Hz]
C4'-H4'	6.80	-13.96
C1-H1	29.63	25.80
C2-H2	30.36	25.59
C5-H5	30.49	25.53
C7-H7	-7.72	-8.60
CH_2-**C**H_3	-0.24	-0.25
C4'-P	-0.07	-0.07
C1'-P	0.76	-1.20
C1-P	0.72	-0.48
C2-P	-0.25	-0.14
R		0.912

Table S6: Theoretical (calculated) RDCs of the low-energy **3-SR** conformers normalized against the 3A experimental dataset

Atoms	Experimental RDCs [Hz]	Theoretical Normalized RDCs [Hz]					
		Conformer					
		A	B	C	D	E	F
C4'-H4'	1.76	-9.90	-11.12	-17.91	-19.13	-15.38	-14.09
C1-H1	24.13	22.68	20.88	24.12	24.09	21.72	22.38
C2-H2	25.48	22.42	20.60	24.31	23.46	21.67	21.50
C5-H5	25.63	23.62	20.39	25.75	23.28	21.36	22.10
C7-H7	-5.17	-9.40	-19.37	2.55	-2.32	-13.68	-11.60
CH_2-**C**H_3	-0.09	0.08	-1.88	2.38	-0.23	-0.03	-1.07
C5-C8	-0.58	-1.48	-0.09	-2.16	-0.50	-0.48	-0.99
C4'-P	-0.01	-0.06	-0.06	-0.10	-0.10	-0.08	-0.08
C1'-P	0.21	-1.01	-0.87	-1.94	-1.64	-1.23	-1.24
C1-P	0.55	-0.47	-0.62	-0.54	-0.58	-0.51	-0.13
C2-P	-0.21	-0.09	-0.14	-0.06	-0.09	-0.11	-0.17
R		0.963	0.921	0.875	0.886	0.917	0.933
Q		0.509	0.611	0.350	0.552	0.637	0.628

Table S7: Theoretical (calculated) RDCs of the low-energy **3-SR** conformers normalized against the 3B experimental dataset

Atoms	Experimental RDCs [Hz]	Theoretical Normalized RDCs [Hz]					
		Conformer					
		A	B	C	D	E	F
C4'-H4'	6.80	-12.17	-13.31	-23.05	-24.16	-18.84	-17.32
C1-H1	29.63	27.87	24.99	31.04	30.42	26.61	27.52
C2-H2	30.36	27.55	24.65	31.29	29.63	26.55	26.44
C5-H5	30.49	29.03	24.39	33.14	29.40	26.17	27.17
C7-H7	-7.72	-11.56	-23.17	3.28	-2.93	-16.75	-14.26
CH_2-**C**H_3	-0.24	0.10	-2.25	3.06	-0.30	-0.04	-1.31
C4'-P	-0.07	-0.07	-0.07	-0.13	-0.13	-0.10	-0.09
C1'-P	0.76	-1.25	-1.04	-2.49	-2.07	-1.51	-1.52
C1-P	0.72	-0.58	-0.74	-0.70	-0.73	-0.63	-0.15
C2-P	-0.25	-0.11	-0.17	-0.08	-0.12	-0.13	-0.21
R		0.935	0.910	0.814	0.833	0.887	0.901
Q		0.506	0.619	0.352	0.564	0.650	0.638

Table S8: Boltzmann distribution-weight averaged RDCs of **3-SR** conformers normalized against the 3A experimental dataset

Atoms	Experimental RDCs [Hz]	Normalized Boltzmann averaged RDCs [Hz]
C4'-H4'	1.76	-10.57
C1-H1	24.13	21.22
C2-H2	25.48	20.96
C5-H5	25.63	21.74
C7-H7	-5.17	-10.03
CH_2-**C**H_3	-0.09	-0.23
C5-C8	-0.58	-1.10
C4'-P	-0.01	-0.06
C1'-P	0.21	-1.01
C1-P	0.55	-0.48
C2-P	-0.21	-0.10
R		0.954

Table S9: Boltzmann distribution-weight averaged RDCs of **3-SR** conformers normalized against the 3B experimental dataset

Atoms	Experimental RDCs [Hz]	Normalized Boltzmann averaged RDCs [Hz]
C4'-H4'	6.80	-13.00
C1-H1	29.63	26.04
C2-H2	30.36	25.73
C5-H5	30.49	26.69
C7-H7	-7.72	-12.21
CH_2-**C**H_3	-0.24	-0.26
C4'-P	-0.07	-0.07
C1'-P	0.76	-1.25
C1-P	0.72	-0.58
C2-P	-0.25	-0.12
R		0.925

2. MDOC Simulations

2.1. Parametrization of MDOC

MDOC stands for molecular dynamics with orientational constraints. These simulations use the COSMOS-NMR force field[21, 22] and two types of constraints from NMR measurements,[23] namely tensor constraints, such as NMR dipole-dipole tensors from RDC measurements, and scalar constraints, such as distances from NOE measurements or ^3J couplings.[24, 25] The tensor constraints cause molecular rotations of the molecules and their mobile groups.

Table S10: General parameters of MDOC simulations

Parameter	Value
Target temperature Compound **3**	290 K 265 K
MD time step	0.5 fs
BPT atomic charge calculation	2.0 fs
Coupling time η to the heat bath	0.02 ps
Memory decay time τ for the property average	200 ps
Time constant ρ for the exponential rise of pseudo-forces	200 ps
Order parameter of the alignment medium S_{am} (dipolar couplings)	0.004
Total MD duration	40 ns

Table S11: Width and weight parameters of pseudo-forces in MDOC simulations

Parameter	Value
Pseudo-force width ΔD for the one bond C-H couplings	0.5 Hz
Weight parameter k_D (one bond couplings [kJ mol^{-1} Hz^{-1}])	0.003
Pseudo-force width ΔD for the other RDC	0.2
Weight parameter k_D [kJ mol^{-1} Hz^{-1}]	0.01
Pseudo-force width ΔJ for the $^3J_{H\text{-}H}$ coupling constraints	2.0 Hz
Weight parameter k_J ($^3J_{H\text{-}H}$ couplings [kJ mol^{-1} Hz^{-1}])	12

2.2. Results of the compounds 1-SR and 1-RR

Table S2: The χ-Probability and n/χ2 values of compounds **1** with different datasets

Dataset	Structure	χ-Probability [%]	n/χ2
1A	1-SR	90.3	0.1948
1A	1-RR	9.7	0.1304
1B	1-SR	52.9	0.1176
1B	1-RR	47.1	0.1116
1A+^3J	1-SR	95.9	0.2160
1A+^3J	1-RR	4.1	0.1366
1B+^3J	1-SR	2.8	0.06977
1B+^3J	1-RR	97.2	0.1201

Based on the χ-Probability, dataset 1A with ^3J couplings has a 95.5% probability of belonging to the structure **1-SR**, and dataset 1B with ^3J couplings has a 97.2 % probability of belonging to the structure **1-RR**.

Table S11: MDOC-simulated data of compound **1-SR** with the assigned dataset 1A

Atoms		RDC calculated [Hz]	RDC experimental [Hz]	Difference [Hz]	Error [Hz]
C1	P	0.297	0.46	0.163	0.05
C2	P	0.1045	0.17	0.065	0.05
H2	C2	-9.658	-9.75	-0.092	0.06
C3	P	-0.0364	-0.01	0.026	0.05
C4	P	-0.04	-0.09	-0.05	0.05
C5	P	-0.0953	-0.17	-0.075	0.05
C1'	P	-1.342	-1.54	-0.198	0.05
C4'	P	-0.073	0.1	0.173	0.05
H4'	C4'	-15.0295	-15.1	-0.07	0.12

Table S12: MDOC-simulated data of compounds **1-RR** with the assigned dataset 1B

Atoms		RDC calculated [Hz]	RDC experimental [Hz]	Difference [Hz]	Error [Hz]
C2	P	0.1088	0.37	0.261	0.05
H2	C2	-10.0875	-10.16	-0.073	0.07
C3	P	0.0383	0.04	0.002	0.05
C4	P	-0.0222	-0.23	-0.208	0.05
C5	P	-0.0934	-0.34	-0.247	0.05
C1'	P	-0.6886	-0.75	-0.061	0.05
C4'	P	-0.0373	-0.02	0.017	0.05
H4'	C4'	-7.3303	-7.35	-0.02	0.07

Table S13: MDOC-simulated ^{3}J couplings of compounds **1-SR** and **1-RR** with the assigned datasets and the assigned prochiral protons

Dataset Compound	Atoms		^{3}J MDOC calc. [Hz]	^{3}J exp. [Hz]	Error +Error calc. [Hz]
1A **1-SR**	H2	H1A proS	6.871	6.6	1.06
1B	H2	H1B proR	5.534	4.3	0.72
1-RR	H2	H1A proS	8.463	6.4	0.67

2.3. Results of the compounds 2-RR and 2-RS

Table S14: The χ-Probability and n/χ2 values of compounds **2-RS** and **2-RR** with different datasets

Dataset	Structure	χ-Probability [%]	n/χ2
2A	2-RR	37.4	0.1957
2A	2-RS	62.6	0.2157
2B	2-RR	12.6	0.1435
2B	2-RS	87.4	0.1872
2A+^3J	2-RR	72.2	0.2071
2A+^3J	2-RS	27.8	0.1995
2B+^3J	2-RR	14.6	0.1635
2B+^3J	2-RS	85.4	0.2043

Based on the χ-Probability, dataset 2A with ^3J couplings has a 72.2% probability of belonging to the structure **2-RR**, and dataset 2B with ^3J couplings has a 85.4% probability of belonging to the structure **2-RS**.

Table S15: MDOC-simulated data of compound **2-RR** with the assigned dataset 2A

Atoms		RDC calculated [Hz]	RDC experimental [Hz]	Difference [Hz]	Error [Hz]
C1	P	0.5917	0.87	0.278	0.05
C2	P	0.2173	0.41	0.193	0.05
H2	C2	-17.0653	-17.16	-0.095	0.04
C3	P	-0.0052	-0.07	-0.065	0.05
C4	P	-0.0478	-0.14	-0.092	0.05
C5	P	-0.1222	-0.07	0.052	0.05
C3'	P	-0.0699	-0.11	-0.04	0.05
H3'	C3'	-8.6162	-8.64	-0.024	0.18
C4'	P	-0.0443	-0.21	-0.166	0.05
H4'	C4'	-13.8304	-13.93	-0.1	0.18
C5'	P	-0.0378	-0.02	0.018	0.05
H5'	C5'	14.5046	14.56	0.055	1.28
C6'	P	-0.0937	-0.16	-0.066	0.05
H6'	C6'	-9.9651	-10.03	-0.065	0.36

Table S16: MDOC-simulated data of compound **2-RS** with the assigned dataset 2B

Atoms		RDC calculated [Hz]	RDC experimental [Hz]	Difference [Hz]	Error [Hz]
C2	P	0.1963	0.21	0.014	0.05
C1	P	0.5041	0.86	0.356	0.05
C5	P	-0.2134	-0.29	-0.077	0.05
C4	P	-0.0613	-0.21	-0.149	0.05
C6	P	0	0	0	0.05
C4'	P	0.0035	-0.07	-0.074	0.05
C5'	P	0.0077	-0.04	-0.048	0.05
C6'	P	0.0171	0.08	0.063	0.05
H3'	C3'	-7.2009	-7.25	-0.049	0.03
H3'	C3'	-4.5282	-4.55	-0.022	0.06
H4'	C4'	1.8554	1.86	0.005	0.13
H5'	C5'	-1.0748	-1.08	-0.005	0.17
H6'	C6'	-4.4204	-4.44	-0.02	0.17

Table S17: MDOC-simulated ^{3}J couplings of compounds **2-RR** and **2-RS** with the assigned datasets 2A and 2B and the assigned prochiral protons

Dataset Compound	Atoms		^{3}J MDOC calc. [Hz]	^{3}J exp. [Hz]	Error +Error calc. [Hz]
2A					
2-RR	H2	H1B proR	5.796	6.6	0.82
2B	H2	H1B proR	4.485	6.6	1.06
2-RS	H2	H1A proS	9.101	9.0	1.36

2.4. Results of compounds 3-RR and 3-SR

Table S18: χ-Probability and n/χ2 values of compounds **3-RR** and **3-SR** with different datasets

Dataset	Structure	χ-Probability [%]	n/χ2
3A	3-RR	8.05	2.406
3A	3-SR	46.94	2.579
3B	3-RR	20.39	1.323
3B	3-SR	79.61	1.437
3A-ex	3-RR	18.14	2.472
3A-ex	3-SR	26.87	2.519

3A-ex: The dataset 3A-ex was introduced to solve the uncertainty in the assignment of $^{3}J_{H-H}$-couplings. In the dataset 3A-ex, $^{3}J_{H-H}$-couplings of the CH_3 protons of the groups C8a and C8b to H7 were interchanged with respect to the dataset 3A.

The χ-probability did not allow a final assignment. Only a preliminary assignment was performed using the P-C1 RDC: dataset 3B was assigned to the structure **3-SR**, but dataset 3A was not assigned. The highest score of **3-RR** was derived from 3A-ex. Inspecting this value, we observed that in dataset 3B the value is lower (-0.72 Hz) than the value of dataset 3A or 3A-ex (-0.55 Hz). The assignment to the other datasets 3A and 3A-ex is inconclusive mainly because of the outlier of the P-C1 RDCs. If we preliminary assign **3-SR** to data set 3B and **3-RR** to 3A or 3A-ex (3A-ex was selected because of the larger χ-probability) we get the same trend in the simulated RDC values (-0.552 < -0.469).

Table S19: MDOC-simulated RDC data of compound **3-RR** and the dataset 3Aex

Atoms		RDC calculated [Hz]	RDC experimental [Hz]	Difference [Hz]	Error [Hz]
C1	P	-0.4689*	-0.550	-0.081*	0.05
C2	P	-0.2209	-0.210	0.011	0.05
H1	C1	24.0717	24.130	0.058	0.34
H2	C2	25.3593	25.480	0.121	0.32
H5	C5	25.5498	25.630	0.080	0.38
H8a_1	C8a	1.4096	1.450	0.040	0.06
H8a_3	C8a	1.4178	1.450	0.032	0.06
C7	H7	-5.1401	-5.170	-0.030	0.04
H8a_2	C8a	1.4341	1.450	0.016	0.06
C8b	H8b_3	-0.4558	-0.450	0.006	0.06
C8b	H8b_1	-0.4620	-0.450	0.012	0.06
C8b	H8b_2	-0.4645	-0.450	0.014	0.06
C11	H11_2	-0.5744	-0.580	-0.006	0.17
C11	H11_3	-0.5818	-0.580	0.002	0.17
C11	H11_1	-0.5791	-0.580	-0.001	0.17
C4'	H4'	1.7407	1.760	0.019	0.23
C4'	P	0.0154	0.010	-0.005	0.05
C1'	P	0.2386	0.210	-0.029	0.05
H10_2	C10	-0.0902	-0.090	0.000	0.01
H10_3	C10	-0.0909	-0.090	0.001	0.01
H10_1	C10	-0.0904	-0.090	0.000	0.01

*Outlier

Table S20: MDOC simulated RDC data of compound **3-SR** and the dataset 3B

Atoms		RDC calculated [Hz]	RDC experimental [Hz]	Difference [Hz]	Error [Hz]
C1p	P	0.7746	0.760	-0.015	0.05
C1	P	-0.5519*	-0.720	-0.168*	0.05
C2	P	-0.2399	-0.250	-0.010	0.05
C4p	P	0.0475	0.070	0.022	0.05
H1	C1	29.5381	29.630	0.092	0.17
H2	C2	30.2137	30.360	0.146	0.22
H5	C5	30.4000	30.490	0.090	0.15
H8a_1	C8a	-0.5559	-0.540	0.016	0.14
H8a_3	C8a	-0.5523	-0.540	0.012	0.14
C7	H7	-7.6763	-7.720	-0.044	0.14
H8a_2	C8a	-0.5478	-0.540	0.008	0.14
C8b	H8b_3	-0.5534	-0.540	0.013	0.14
C8b	H8b_1	-0.5590	-0.540	0.019	0.14
C8b	H8b_2	-0.5604	-0.540	0.020	0.14
H4p	C4p	6.7860	6.800	0.014	0.30
H10_2	C10	-0.2409	-0.240	0.001	0.08
H10_3	C10	-0.2397	-0.240	-0.000	0.08
H10_1	C10	-0.2363	-0.240	-0.004	0.08

*Outlier

Table S21: MDOC-simulated $^{3}J_{H\text{-}H}$-couplings calculated from the MDOC trajectory of the compound **3-RR** and the dataset 3A-ex

Atoms		^{3}J calculated [Hz]	^{3}J experimental [Hz]	Difference [Hz]	Error [Hz]
H7	H8a_2	6.659	6.900	-0.241	0.68
H7	H8a_3	6.659	6.900	-0.241	0.68
H7	H8a_1	6.624	6.900	-0.276	0.68
H7	H8b_3	6.699	7.100	-0.401	0.68
H7	H8b_1	6.706	7.100	-0.394	0.68
H7	H8b_2	6.691	7.100	-0.409	0.68
H9_2	H10_1	6.263	7.100	-0.837	0.66
H9_2	H10_3	6.226	7.100	-0.874	0.66
H9_2	H10_2	6.302	7.100	-0.798	0.66
H9_1	H10_1	6.513	7.100	-0.587	0.66
H9_1	H10_3	6.534	7.100	-0.566	0.66
H9_1	H10_2	6.507	7.100	-0.593	0.66

Rotating CH_3 groups

Table 22: MDOC-simulated $^{3}J_{H\text{-}H}$-couplings calculated from the MDOC trajectory of compound **3-SR** and the dataset 3B

Atoms		^{3}J calculated [Hz]	^{3}J experimental [Hz]	Difference [Hz]	Error [Hz]
H7	H8a_2	6.723	7.1	-0.377	0.7
H7	H8a_3	6.734	7.1	-0.366	0.7
H7	H8a_1	6.712	7.1	-0.388	0.7
H7	H8b_3	6.707	7.1	-0.393	0.7
H7	H8b_1	6.706	7.1	-0.394	0.7
H7	H8b_2	6.693	7.1	-0.407	0.7
H9_2	H10_1	6.286	7.1	-0.814	0.68
H9_2	H10_3	6.251	7.1	-0.849	0.68
H9_2	H10_2	6.322	7.1	-0.778	0.68
H9_1	H10_1	6.498	7.1	-0.602	0.68
H9_1	H10_3	6.522	7.1	-0.578	0.68
H9_1	H10_2	6.498	7.1	-0.602	0.68

Rotating CH_3 groups

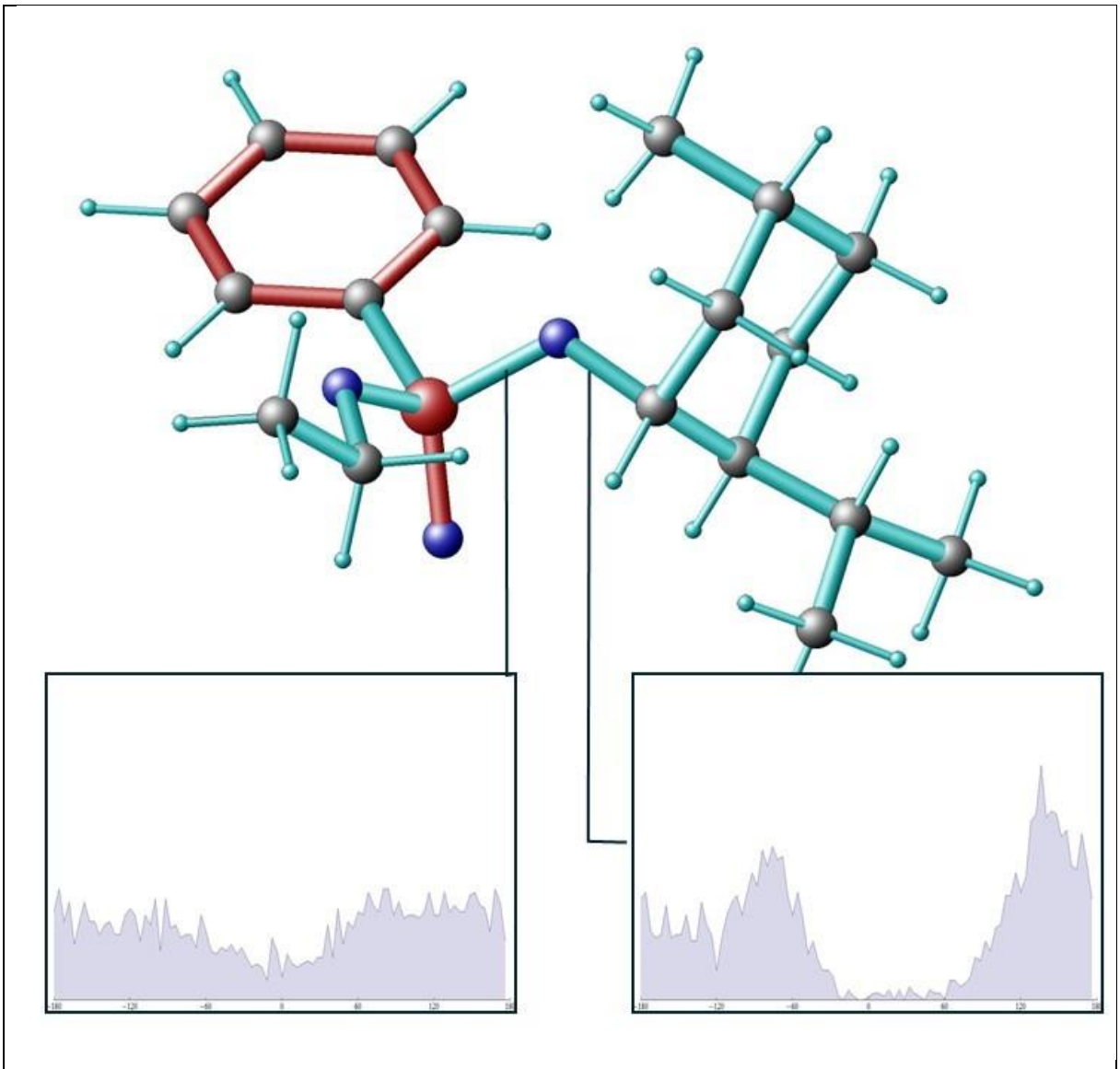


Figure S7: Mobility of the menthol ring system extracted from a MDOC trajectory (**3-RR**-3A-ex) of the torsion around the (C1'-**P-O**-C1) (left panel) and the (P-**O-C1**-C2) (right panel) angles.

3. XYZ coordinates of low energy structures of 3

3-RR - A

P	-0.58853	-2.72199	-3.34069
O	0.33590	-1.94614	-4.21650
O	0.14151	-3.92190	-2.52326
C	-1.98837	-3.45204	-4.21256
C	1.18550	-4.71260	-3.16875
C	2.32369	-4.92168	-2.16171
C	3.38713	-5.83125	-2.81263
C	2.79239	-7.16256	-3.29526
C	1.63018	-6.95131	-4.27898
C	0.57520	-6.03038	-3.64424
C	2.87842	-3.59086	-1.58752
C	3.47828	-2.64985	-2.64589
C	3.88064	-3.84187	-0.44905
C	1.01126	-8.27795	-4.73235
C	-2.94167	-4.22824	-3.53595
C	-3.98612	-4.82004	-4.24591
C	-4.07988	-4.64320	-5.63154
C	-3.13069	-3.87124	-6.30666
C	-2.08405	-3.27369	-5.59905
O	-1.30968	-1.93982	-2.13102
C	-0.49940	-1.28622	-1.11395
C	-0.52416	-2.09873	0.16977
H	1.55972	-4.14580	-4.02896
H	1.88899	-5.47480	-1.31371
H	4.19538	-6.02504	-2.10012
H	3.84140	-5.31146	-3.66681
H	3.57274	-7.77489	-3.76483
H	2.42370	-7.73271	-2.42916
H	2.03304	-6.43927	-5.16721
H	-0.23143	-5.82208	-4.35646
H	0.11707	-6.53239	-2.78046
H	2.01577	-3.07730	-1.14693
H	3.83252	-1.72892	-2.16843
H	2.74446	-2.36151	-3.40426
H	4.34033	-3.10564	-3.14664
H	4.12520	-2.90287	0.05989
H	3.47538	-4.53363	0.29934
H	4.82141	-4.26289	-0.82160
H	0.19968	-8.11367	-5.45021
H	1.75935	-8.92183	-5.20862
H	0.59560	-8.82391	-3.87611
H	-2.86240	-4.36721	-2.46223
H	-4.72526	-5.41931	-3.72229
H	-4.89329	-5.10698	-6.18235
H	-3.20460	-3.73265	-7.38128
H	-1.33782	-2.67102	-6.10746
H	0.52062	-1.14750	-1.48834
H	-0.94635	-0.29800	-0.97562
H	-1.55137	-2.21580	0.52848
H	-0.09818	-3.09083	0.00032
H	0.05900	-1.59013	0.94586

3-RR - B

P	-0.58776	-2.83475	-3.19856
O	0.29773	-1.97531	-4.03606
O	0.18046	-4.06869	-2.47664
C	-1.98949	-3.53652	-4.09088
C	1.22531	-4.79530	-3.19240
C	2.39319	-5.03754	-2.22775
C	3.46006	-5.87925	-2.95937
C	2.88385	-7.19315	-3.50784
C	1.69168	-6.95135	-4.44770
C	0.63278	-6.09637	-3.73223
C	2.93066	-3.73094	-1.58566
C	3.48325	-2.71269	-2.59720
C	3.96644	-4.02652	-0.48854
C	1.09149	-8.26294	-4.96553
C	-2.12658	-3.25551	-5.45676
C	-3.17597	-3.82602	-6.18243
C	-4.08699	-4.67295	-5.54570
C	-3.95197	-4.95242	-4.18054
C	-2.90443	-4.38810	-3.45295
O	-1.30005	-2.15014	-1.92457
C	-0.47898	-1.49438	-0.92011
C	-1.38466	-0.59991	-0.09576
H	1.56556	-4.16965	-4.02567
H	1.99283	-5.65177	-1.40543
H	4.29105	-6.09614	-2.28043
H	3.87965	-5.29753	-3.79110
H	3.66548	-7.75652	-4.03328
H	2.55123	-7.82368	-2.66943
H	2.05935	-6.37707	-5.31285
H	-0.19653	-5.86535	-4.41061
H	0.20892	-6.66058	-2.88966
H	2.06633	-3.26666	-1.09563
H	3.82781	-1.81456	-2.07164
H	2.72497	-2.39564	-3.31912
H	4.34321	-3.11603	-3.14453
H	4.20104	-3.11492	0.07232
H	3.59682	-4.77362	0.22425
H	4.90764	-4.39928	-0.90850
H	0.71085	-8.86939	-4.13407
H	0.25791	-8.07556	-5.65185
H	1.84137	-8.85861	-5.49835
H	-1.40991	-2.59547	-5.93564
H	-3.28168	-3.60821	-7.24114
H	-4.90249	-5.11571	-6.11056
H	-4.66133	-5.61010	-3.68669
H	-2.79273	-4.60700	-2.39554
H	-0.00920	-2.26921	-0.30444
H	0.30574	-0.91685	-1.42109
H	-0.80314	-0.10310	0.68840
H	-1.84675	0.16501	-0.72648
H	-2.17803	-1.18624	0.37765

3-RR - C

P	-0.40944	-3.25928	-3.99474
O	0.02241	-2.80005	-5.34584
O	0.14106	-4.66936	-3.45638
C	-2.19228	-3.46617	-3.81267
C	1.58224	-4.91989	-3.40782
C	1.89976	-5.61058	-2.07549
C	3.39050	-6.00927	-2.07112
C	3.76286	-6.88156	-3.27838
C	3.43239	-6.18337	-4.60766
C	1.95169	-5.77012	-4.62132
C	1.45744	-4.78232	-0.83963
C	2.28584	-3.50710	-0.61337
C	1.43568	-5.64280	0.43409
C	3.77594	-7.05766	-5.81852
C	-3.01778	-3.18357	-4.90879
C	-4.40461	-3.30317	-4.78441
C	-4.96558	-3.70493	-3.56917
C	-4.14128	-3.98940	-2.47403
C	-2.75674	-3.86920	-2.59287
O	0.07869	-2.27799	-2.78946
C	0.20411	-0.84999	-3.01015
C	-1.12071	-0.13589	-2.78379
H	2.10674	-3.95769	-3.45917
H	1.30488	-6.53715	-2.06896
H	3.62926	-6.53516	-1.14049
H	4.01140	-5.10343	-2.08495
H	4.82998	-7.13565	-3.24384
H	3.21060	-7.83205	-3.22929
H	4.04059	-5.26643	-4.66377
H	1.70863	-5.21087	-5.53116
H	1.31940	-6.66887	-4.61243
H	0.42665	-4.46760	-1.03910
H	1.84700	-2.91452	0.19703
H	2.30520	-2.87222	-1.50344
H	3.31784	-3.74053	-0.32785
H	2.44311	-5.96110	0.72660
H	1.01710	-5.07739	1.27438
H	0.82496	-6.54308	0.29823
H	4.83739	-7.33068	-5.82140
H	3.19100	-7.98585	-5.80407
H	3.55677	-6.53873	-6.75830
H	-2.56564	-2.87357	-5.84594
H	-5.04402	-3.08487	-5.63470
H	-6.04368	-3.79812	-3.47363
H	-4.57829	-4.30358	-1.53066
H	-2.11441	-4.08844	-1.74552
H	0.95735	-0.52351	-2.28734
H	0.58691	-0.67940	-4.02146
H	-0.97912	0.94706	-2.87181
H	-1.86682	-0.44463	-3.52222
H	-1.51187	-0.35745	-1.78611

3-RR – D

P	-0.31502	-3.21303	-3.90941
O	0.30098	-2.78542	-5.19784
O	0.20031	-4.58104	-3.24524
C	-2.10207	-3.45598	-3.98719
C	1.62670	-4.92145	-3.26037
C	1.95425	-5.69710	-1.97845
C	3.40533	-6.22461	-2.07912
C	3.66446	-7.04571	-3.34792
C	3.33687	-6.24157	-4.61453
C	1.89130	-5.73009	-4.53161
C	1.73706	-4.93113	-0.64118
C	0.26035	-4.80567	-0.22646
C	2.41323	-3.54915	-0.59905
C	3.56533	-7.05625	-5.89226
C	-2.75650	-3.22555	-5.20490
C	-4.14199	-3.38635	-5.29243
C	-4.87282	-3.77754	-4.16748
C	-4.22057	-4.00776	-2.95052
C	-2.83816	-3.84574	-2.85740
O	-0.05112	-2.18068	-2.67654
C	-0.21962	-0.75823	-2.90159
C	0.26963	-0.03612	-1.65998
H	2.20796	-3.99179	-3.28959
H	1.28597	-6.57161	-1.96755
H	3.62230	-6.82678	-1.18863
H	4.10470	-5.37769	-2.05722
H	4.70945	-7.38048	-3.37154
H	3.04226	-7.95320	-3.33290
H	4.00671	-5.36729	-4.64093
H	1.64689	-5.10564	-5.39693
H	1.20016	-6.58472	-4.53803
H	2.22478	-5.55779	0.12053
H	0.18999	-4.48466	0.81969
H	-0.26631	-5.76184	-0.32300
H	-0.25739	-4.06641	-0.83972
H	2.35460	-3.13329	0.41318
H	3.47228	-3.59444	-0.87382
H	1.90901	-2.84738	-1.26971
H	2.91479	-7.93973	-5.90931
H	3.34649	-6.46223	-6.78648
H	4.60286	-7.40291	-5.96051
H	-2.17353	-2.92435	-6.06984
H	-4.64783	-3.20825	-6.23683
H	-5.94958	-3.90377	-4.23675
H	-4.78910	-4.31327	-2.07698
H	-2.33111	-4.02712	-1.91511
H	0.35022	-0.47043	-3.79113
H	-1.28246	-0.55304	-3.08558
H	0.14716	1.04516	-1.78369
H	-0.29783	-0.35357	-0.77990
H	1.32812	-0.24931	-1.48365

3-RR – E

P	-0.32476	-3.27426	-4.01423
O	0.04158	-2.93235	-5.41839
O	0.24824	-4.63914	-3.38477
C	-2.09946	-3.45570	-3.73987
C	1.68347	-4.86746	-3.21378
C	1.87193	-5.95790	-2.15092
C	3.38701	-6.23071	-2.01285
C	4.04952	-6.60241	-3.34599
C	3.81327	-5.53194	-4.42244
C	2.30722	-5.25412	-4.55639
C	1.21887	-5.67152	-0.76752
C	-0.26209	-6.08271	-0.71380
C	1.40413	-4.22256	-0.28595
C	4.42778	-5.92598	-5.77004
C	-2.94452	-3.58182	-4.85049
C	-4.32300	-3.71442	-4.66428
C	-4.85757	-3.71737	-3.37290
C	-4.01516	-3.58372	-2.26326
C	-2.63841	-3.45148	-2.44446
O	0.20561	-2.19505	-2.91574
C	0.34309	-0.79480	-3.27387
C	-0.96735	-0.04375	-3.08873
H	2.12790	-3.93016	-2.85661
H	1.40835	-6.87117	-2.55326
H	3.53646	-7.03554	-1.28331
H	3.88018	-5.34023	-1.59704
H	5.12594	-6.76060	-3.20126
H	3.63592	-7.55785	-3.70229
H	4.29885	-4.60251	-4.08375
H	2.12156	-4.45826	-5.28423
H	1.79622	-6.15334	-4.92774
H	1.74956	-6.31896	-0.05374
H	-0.66459	-5.93879	0.29617
H	-0.38594	-7.14032	-0.97470
H	-0.86287	-5.49799	-1.41259
H	0.83405	-3.51924	-0.90010
H	1.05911	-4.12230	0.74927
H	2.45581	-3.91465	-0.31186
H	4.27191	-5.14415	-6.52154
H	5.50617	-6.09909	-5.67807
H	3.97097	-6.84908	-6.14817
H	-2.51584	-3.56655	-5.84779
H	-4.97732	-3.81262	-5.52550
H	-5.92950	-3.81971	-3.22955
H	-4.43131	-3.58081	-1.26006
H	-1.98390	-3.33732	-1.58626
H	1.11720	-0.41201	-2.60295
H	0.70268	-0.72735	-4.30541
H	-1.33735	-0.15834	-2.06527
H	-0.81427	1.02284	-3.28745
H	-1.73442	-0.41311	-3.77597

3-RR – F

P	-0.50623	-3.45180	-4.22568
O	-0.17666	-3.50197	-5.67915
O	0.05375	-4.63545	-3.28482
C	-2.26968	-3.49692	-3.85199
C	1.48701	-4.82767	-3.07664
C	1.68420	-5.62162	-1.77886
C	3.19963	-5.86286	-1.59325
C	3.84717	-6.55268	-2.80122
C	3.60374	-5.77543	-4.10394
C	2.09696	-5.53459	-4.28875
C	1.05109	-4.99173	-0.50423
C	-0.43378	-5.35469	-0.33511
C	1.25873	-3.47106	-0.40076
C	4.20690	-6.48661	-5.32014
C	-3.15772	-3.91432	-4.85237
C	-4.52855	-3.96695	-4.58708
C	-5.01225	-3.59999	-3.32826
C	-4.12673	-3.17437	-2.33161
C	-2.75716	-3.12088	-2.59122
O	0.07254	-2.13239	-3.46742
C	0.64506	-1.03312	-4.22353
C	2.15068	-1.20232	-4.34811
H	1.94214	-3.83573	-2.96456
H	1.21056	-6.60246	-1.93480
H	3.35390	-6.46574	-0.69047
H	3.70102	-4.90105	-1.41264
H	4.92439	-6.67717	-2.63182
H	3.42657	-7.56359	-2.91042
H	4.09295	-4.79282	-4.00459
H	1.90408	-4.94189	-5.18846
H	1.58161	-6.49550	-4.42438
H	1.58384	-5.44839	0.34310
H	-0.81880	-4.96351	0.61434
H	-0.57427	-6.44193	-0.32942
H	-1.03844	-4.94763	-1.14745
H	0.92991	-3.11115	0.58050
H	2.31306	-3.19344	-0.51470
H	0.68712	-2.93492	-1.16406
H	4.04498	-5.91066	-6.23801
H	5.28592	-6.63482	-5.19756
H	3.74651	-7.47273	-5.45892
H	-2.76878	-4.18695	-5.82857
H	-5.21643	-4.29125	-5.36237
H	-6.07833	-3.64098	-3.12360
H	-4.50367	-2.88365	-1.35542
H	-2.06905	-2.78358	-1.82268
H	0.17439	-0.98333	-5.20990
H	0.38722	-0.13370	-3.65746
H	2.61152	-1.29584	-3.35952
H	2.58598	-0.33259	-4.85295
H	2.38582	-2.09431	-4.93626

3-RR – G

P	-0.28880	-3.21155	-3.80292
O	0.24588	-2.78385	-5.12785
O	0.23902	-4.59675	-3.18407
C	-2.07990	-3.43375	-3.76647
C	1.66303	-4.93923	-3.25442
C	2.03690	-5.73357	-1.99671
C	3.48062	-6.26566	-2.16015
C	3.68831	-7.06926	-3.44935
C	3.31761	-6.24491	-4.69078
C	1.87825	-5.72991	-4.54643
C	1.87579	-4.98600	-0.64126
C	2.56655	-3.61099	-0.60173
C	0.41667	-4.85231	-0.17108
C	3.49520	-7.04088	-5.98822
C	-2.74942	-3.83612	-2.60093
C	-4.13839	-3.96513	-2.60681
C	-4.86341	-3.69032	-3.77215
C	-4.19794	-3.28997	-4.93391
C	-2.80639	-3.16197	-4.93370
O	0.08492	-2.18850	-2.59143
C	0.17039	-0.76060	-2.83604
C	-1.19014	-0.09172	-2.70185
H	2.24510	-4.01012	-3.29105
H	1.36545	-6.60538	-1.97175
H	3.72842	-6.88132	-1.28710
H	4.18429	-5.42209	-2.15286
H	4.73011	-7.40797	-3.51674
H	3.06285	-7.97428	-3.42451
H	3.98977	-5.37279	-4.72882
H	1.60342	-5.09242	-5.39293
H	1.18426	-6.58218	-4.53962
H	2.38453	-5.62908	0.09251
H	2.04519	-2.89464	-1.24380
H	3.61469	-3.66099	-0.91461
H	2.54779	-3.21113	0.41839
H	0.38740	-4.55341	0.88349
H	-0.11209	-4.09276	-0.74909
H	-0.12605	-5.79916	-0.26995
H	3.24577	-6.43262	-6.86468
H	4.52806	-7.39012	-6.10012
H	2.84087	-7.92168	-5.99442
H	-2.18746	-4.05104	-1.69796
H	-4.65561	-4.27917	-1.70485
H	-5.94513	-3.79019	-3.77310
H	-4.75946	-3.07945	-5.83940
H	-2.27421	-2.85334	-5.82828
H	0.86800	-0.39152	-2.07885
H	0.60616	-0.59645	-3.82676
H	-1.08145	0.99375	-2.80428
H	-1.88104	-0.44113	-3.47491
H	-1.63055	-0.30818	-1.72379

3-RR – H

P	-0.43743	-2.85090	-3.29362
O	0.33881	-2.10925	-4.32845
O	0.40744	-4.00435	-2.52426
C	-1.94083	-3.64155	-3.90229
C	1.46199	-4.73666	-3.22044
C	2.39943	-5.34091	-2.16733
C	3.48368	-6.15991	-2.90262
C	2.89206	-7.23183	-3.82747
C	1.91858	-6.63002	-4.85228
C	0.84458	-5.80562	-4.12444
C	3.03030	-4.31875	-1.17771
C	2.12159	-4.03106	0.02982
C	3.48868	-3.01448	-1.85138
C	1.28593	-7.70304	-5.74512
C	-2.68985	-4.50360	-3.08760
C	-3.83225	-5.12183	-3.59641
C	-4.22660	-4.88599	-4.91854
C	-3.47940	-4.02939	-5.73168
C	-2.33606	-3.40549	-5.22561
O	-0.99195	-1.98861	-2.04686
C	-0.13827	-0.98148	-1.43809
C	-0.97698	-0.22158	-0.42888
H	2.01024	-4.01559	-3.83724
H	1.79823	-6.04777	-1.57543
H	4.13983	-6.62789	-2.15909
H	4.11623	-5.48003	-3.49112
H	3.69630	-7.77055	-4.34453
H	2.35282	-7.97614	-3.22218
H	2.49027	-5.94205	-5.49484
H	0.18188	-5.32963	-4.85571
H	0.21847	-6.46699	-3.50942
H	3.93221	-4.80785	-0.78087
H	2.61460	-3.34673	0.73066
H	1.88950	-4.95448	0.57351
H	1.17466	-3.58746	-0.28456
H	2.63995	-2.42556	-2.21202
H	4.04570	-2.39565	-1.13924
H	4.14634	-3.20505	-2.70655
H	2.05226	-8.27200	-6.28373
H	0.70213	-8.41182	-5.14450
H	0.61202	-7.25762	-6.48553
H	-2.37563	-4.69126	-2.06550
H	-4.41293	-5.78874	-2.96576
H	-5.11468	-5.37136	-5.31331
H	-3.78448	-3.84767	-6.75806
H	-1.74087	-2.74275	-5.84635
H	0.70878	-1.47975	-0.95477
H	0.24532	-0.32466	-2.22571
H	-0.36753	0.54937	0.05481
H	-1.82632	0.26169	-0.92067
H	-1.35987	-0.89761	0.34159

3-RS – A

P	-0.94254	3.41337	2.80506
O	0.39454	3.95474	3.18057
O	-0.90947	2.36328	1.56584
C	-1.80575	2.58893	4.15771
C	0.19187	1.40943	1.46411
C	-0.37604	0.07473	0.96362
C	0.79571	-0.90638	0.75096
C	1.86011	-0.34104	-0.20050
C	2.41070	1.00640	0.29427
C	1.25082	1.98816	0.52801
C	-1.51777	-0.47543	1.85799
C	-1.06677	-0.89409	3.26675
C	-2.26958	-1.62732	1.17162
C	3.44969	1.59205	-0.66806
C	-1.12165	2.38703	5.36378
C	-1.73970	1.69292	6.40733
C	-3.03918	1.20472	6.24874
C	-3.72676	1.41304	5.04738
C	-3.11286	2.10289	4.00239
O	-2.05502	4.45054	2.27065
C	-1.75259	5.28312	1.11790
C	-2.91508	6.23773	0.92502
H	0.63277	1.27407	2.46009
H	-0.81921	0.28433	-0.02259
H	0.41608	-1.85760	0.36313
H	1.26623	-1.12948	1.71810
H	2.68044	-1.06065	-0.31779
H	1.42004	-0.19951	-1.19919
H	2.90326	0.83098	1.26384
H	1.61529	2.92908	0.95304
H	0.76774	2.22185	-0.43167
H	-2.22913	0.34975	1.97477
H	-1.93668	-1.16159	3.87567
H	-0.54735	-0.08827	3.79315
H	-0.40335	-1.76576	3.23543
H	-3.15159	-1.91240	1.75619
H	-2.60950	-1.34222	0.16898
H	-1.64272	-2.52112	1.07277
H	3.85013	2.53973	-0.29111
H	4.28945	0.90263	-0.81209
H	3.00183	1.78440	-1.65122
H	-0.11392	2.77630	5.47145
H	-1.20791	1.53544	7.34103
H	-3.51855	0.66399	7.05986
H	-4.73861	1.03713	4.92685
H	-3.64245	2.26584	3.06903
H	-0.81764	5.82161	1.30777
H	-1.61586	4.63288	0.24671
H	-3.04616	6.86792	1.80953
H	-2.72651	6.88328	0.06046
H	-3.84331	5.68496	0.75117

3-RS – B

P	-0.76258	2.71392	3.15947
O	0.42158	2.64636	4.06407
O	-0.95181	1.53714	2.08306
C	-2.34903	2.69249	4.01763
C	0.15062	1.19095	1.18364
C	0.32784	-0.33237	1.20329
C	1.41911	-0.70504	0.17727
C	1.09729	-0.17882	-1.22922
C	0.88853	1.34434	-1.23865
C	-0.18470	1.72697	-0.20605
C	0.55887	-0.90490	2.62713
C	1.85863	-0.42619	3.29504
C	0.47953	-2.44056	2.63153
C	0.53026	1.86738	-2.63393
C	-2.35565	2.58232	5.41450
C	-3.56939	2.58979	6.10704
C	-4.77318	2.70653	5.40684
C	-4.76726	2.81558	4.01124
C	-3.55812	2.81023	3.31570
O	-0.75874	4.02161	2.18779
C	-0.19828	5.27516	2.65968
C	-1.21620	6.07745	3.45793
H	1.06485	1.66983	1.55548
H	-0.62429	-0.75355	0.84359
H	1.54175	-1.79253	0.14694
H	2.38363	-0.29153	0.50112
H	1.90072	-0.45030	-1.92589
H	0.18168	-0.66363	-1.60021
H	1.83654	1.81325	-0.92992
H	-0.30530	2.81385	-0.14840
H	-1.15413	1.30830	-0.51097
H	-0.27561	-0.53681	3.23627
H	1.93629	-0.85028	4.30242
H	1.88604	0.66122	3.40592
H	2.74348	-0.75216	2.73575
H	0.48102	-2.82034	3.65918
H	-0.43516	-2.79817	2.14345
H	1.33502	-2.89375	2.11716
H	0.40727	2.95641	-2.63164
H	1.30888	1.61621	-3.36317
H	-0.41108	1.42492	-2.98328
H	-1.41134	2.49348	5.94282
H	-3.57414	2.50374	7.18966
H	-5.71620	2.71220	5.94609
H	-5.70358	2.90500	3.46816
H	-3.54922	2.89608	2.23348
H	0.69836	5.06164	3.25024
H	0.09602	5.80583	1.75000
H	-0.79419	7.05388	3.72077
H	-2.12683	6.23636	2.87233
H	-1.48830	5.56255	4.38418

3-RS – C

P	-0.91839	3.34973	2.93214
O	0.44348	3.86134	3.25609
O	-0.94405	2.26980	1.71402
C	-1.76264	2.59059	4.33317
C	0.15538	1.32784	1.51810
C	-0.38828	0.09243	0.78545
C	0.79744	-0.85476	0.48819
C	1.92951	-0.17402	-0.29107
C	2.44449	1.07882	0.43265
C	1.26894	2.02213	0.73044
C	-1.54681	-0.66872	1.49202
C	-2.92386	-0.02601	1.25528
C	-1.30658	-0.91010	2.99178
C	3.54317	1.79324	-0.36171
C	-0.99835	2.23423	5.45301
C	-1.60051	1.56959	6.52426
C	-2.96446	1.26822	6.48238
C	-3.73161	1.63684	5.37143
C	-3.13382	2.29566	4.29741
O	-2.02308	4.39804	2.40640
C	-1.79681	5.12133	1.16406
C	-2.63207	4.51547	0.04837
H	0.53979	1.03082	2.50281
H	-0.77294	0.45003	-0.18199
H	0.42509	-1.72113	-0.07146
H	1.19644	-1.24621	1.43462
H	2.75241	-0.88152	-0.45509
H	1.56225	0.11831	-1.28650
H	2.87201	0.75934	1.39641
H	1.60597	2.89462	1.29700
H	0.84107	2.38439	-0.21581
H	-1.57724	-1.65654	1.00855
H	-3.71726	-0.65559	1.67514
H	-2.98613	0.95927	1.71920
H	-3.12254	0.09461	0.18380
H	-1.37564	0.01804	3.56505
H	-2.06402	-1.59332	3.39101
H	-0.32535	-1.35736	3.18471
H	3.16011	2.13371	-1.33206
H	3.91609	2.67077	0.17788
H	4.39156	1.12610	-0.55257
H	0.05775	2.48452	5.47516
H	-1.00673	1.29175	7.39004
H	-3.43177	0.75121	7.31565
H	-4.79325	1.40966	5.34287
H	-3.72566	2.58419	3.43512
H	-2.08773	6.15422	1.37346
H	-0.72863	5.11154	0.92153
H	-2.33085	3.48056	-0.13093
H	-2.49700	5.09148	-0.87422
H	-3.69381	4.53125	0.31354

3-RS – D

P	-0.72642	2.75548	3.13995
O	0.54866	2.86109	3.90614
O	-0.85779	1.53959	2.10043
C	-2.19087	2.53764	4.17147
C	0.26212	1.16191	1.23669
C	0.30570	-0.36792	1.14295
C	1.40995	-0.75728	0.13301
C	1.23163	-0.09076	-1.23730
C	1.16447	1.43991	-1.12251
C	0.06364	1.83040	-0.12394
C	0.48740	-1.12148	2.49315
C	-0.82102	-1.27947	3.28755
C	1.59612	-0.53644	3.38549
C	0.94681	2.11107	-2.48298
C	-2.02210	2.31879	5.54544
C	-3.14034	2.13801	6.36344
C	-4.42388	2.17642	5.81172
C	-4.59386	2.39903	4.44034
C	-3.48036	2.58127	3.61972
O	-1.03255	4.02954	2.17401
C	-0.84744	5.36616	2.70745
C	-1.00131	6.34546	1.55898
H	1.18601	1.52804	1.69998
H	-0.65834	-0.68316	0.71512
H	1.41778	-1.84806	0.02147
H	2.39163	-0.48086	0.54226
H	2.05026	-0.38248	-1.90762
H	0.30094	-0.45137	-1.70081
H	2.12805	1.78864	-0.71799
H	0.02744	2.91608	0.01392
H	-0.91592	1.52499	-0.51782
H	0.80079	-2.13757	2.20962
H	-0.66760	-1.95608	4.13655
H	-1.17847	-0.32450	3.67715
H	-1.61649	-1.70140	2.66206
H	1.77886	-1.19984	4.23829
H	2.54399	-0.43027	2.84605
H	1.32420	0.44645	3.78280
H	0.92371	3.20275	-2.38933
H	1.74516	1.84855	-3.18644
H	-0.00626	1.79268	-2.92371
H	-1.01833	2.29431	5.95830
H	-3.00914	1.96737	7.42790
H	-5.29246	2.03476	6.44857
H	-5.59198	2.43008	4.01324
H	-3.60704	2.75411	2.55527
H	-1.60326	5.54477	3.48361
H	0.14483	5.43026	3.16584
H	-1.99144	6.25345	1.10227
H	-0.87881	7.37104	1.92339
H	-0.24596	6.15636	0.79028

3-RS – E

P	-0.55777	2.76166	3.42180
O	0.67541	2.44970	4.19003
O	-0.84058	1.86093	2.10878
C	-2.10634	2.57126	4.33450
C	0.27152	1.30227	1.34223
C	-0.04695	-0.16759	1.04551
C	1.08461	-0.73760	0.16470
C	1.28325	0.08112	-1.11983
C	1.56754	1.56262	-0.82203
C	0.45621	2.13381	0.07491
C	-0.35066	-0.99042	2.32594
C	0.82339	-1.06681	3.31687
C	-0.86287	-2.39823	1.98043
C	1.72796	2.38709	-2.10384
C	-3.31508	2.24631	3.69979
C	-4.48867	2.13626	4.44874
C	-4.46066	2.34925	5.83043
C	-3.25636	2.66726	6.46604
C	-2.08010	2.77756	5.72203
O	-0.51798	4.29140	2.87453
C	-1.54915	4.81424	2.00505
C	-1.12241	6.20251	1.56553
H	1.17419	1.36765	1.95964
H	-0.96915	-0.16957	0.44230
H	0.86617	-1.77936	-0.09122
H	2.02383	-0.74552	0.73364
H	2.10277	-0.34292	-1.71379
H	0.37682	0.01214	-1.74022
H	2.51268	1.61534	-0.25928
H	0.68246	3.17002	0.35340
H	-0.49392	2.14367	-0.47824
H	-1.17032	-0.46375	2.83042
H	1.68750	-1.57900	2.87764
H	0.52499	-1.63702	4.20377
H	1.14051	-0.07789	3.66062
H	-1.23280	-2.90199	2.88020
H	-1.68463	-2.36148	1.25492
H	-0.07011	-3.02720	1.55921
H	0.80568	2.36355	-2.69796
H	1.95464	3.43522	-1.87763
H	2.53798	1.99394	-2.72840
H	-3.32979	2.06268	2.63040
H	-5.42154	1.87906	3.95549
H	-5.37415	2.26058	6.41150
H	-3.23158	2.82221	7.54064
H	-1.13750	3.00662	6.20988
H	-1.66766	4.14344	1.14618
H	-2.49848	4.84620	2.55442
H	-1.88469	6.63791	0.91035
H	-0.99056	6.85629	2.43248
H	-0.17537	6.15778	1.01959

3-RS – F

P	-1.48813	2.93666	2.51395
O	-0.46197	3.70932	1.75667
O	-1.69413	1.40189	2.02804
C	-1.21260	2.89528	4.29725
C	-0.60889	0.51482	1.61572
C	-0.01399	0.90415	0.25052
C	1.03247	-0.16537	-0.12865
C	2.12083	-0.31074	0.94551
C	1.52836	-0.64783	2.32346
C	0.46443	0.39742	2.69956
C	-1.09139	1.16317	-0.83405
C	-1.97254	-0.05557	-1.15184
C	-0.47135	1.73661	-2.11821
C	2.60899	-0.75104	3.40537
C	-2.04248	2.14564	5.14399
C	-1.78351	2.10632	6.51430
C	-0.69559	2.81163	7.04185
C	0.13135	3.55939	6.19904
C	-0.12583	3.60324	4.82635
O	-3.01343	3.45847	2.42928
C	-3.65183	3.59215	1.13199
C	-4.94188	4.36460	1.33094
H	-1.11908	-0.45079	1.52514
H	0.51347	1.85550	0.39691
H	1.49436	0.09314	-1.08693
H	0.53866	-1.13678	-0.27178
H	2.84185	-1.08387	0.65071
H	2.68209	0.63209	1.02327
H	1.02795	-1.62620	2.24303
H	-0.00928	0.14110	3.65407
H	0.95421	1.37125	2.83222
H	-1.74537	1.94118	-0.42546
H	-2.73927	0.21235	-1.88770
H	-2.48984	-0.43110	-0.26288
H	-1.38681	-0.87835	-1.57773
H	-1.25548	2.06760	-2.80864
H	0.16782	2.59868	-1.89692
H	0.13347	0.99125	-2.64736
H	2.17600	-1.01216	4.37769
H	3.35289	-1.51407	3.14963
H	3.13454	0.20517	3.51916
H	-2.88230	1.59617	4.72993
H	-2.42645	1.52669	7.17033
H	-0.49442	2.77757	8.10886
H	0.97477	4.10755	6.60855
H	0.50872	4.17613	4.15713
H	-2.97179	4.11803	0.45244
H	-3.84130	2.58815	0.73608
H	-4.73522	5.36067	1.73305
H	-5.46155	4.47446	0.37294
H	-5.60211	3.83879	2.02732

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