SUPPORTING INFORMATION

Exploring the impact of alignment media on RDC analysis of phosphorus-containing compounds: A molecular docking approach

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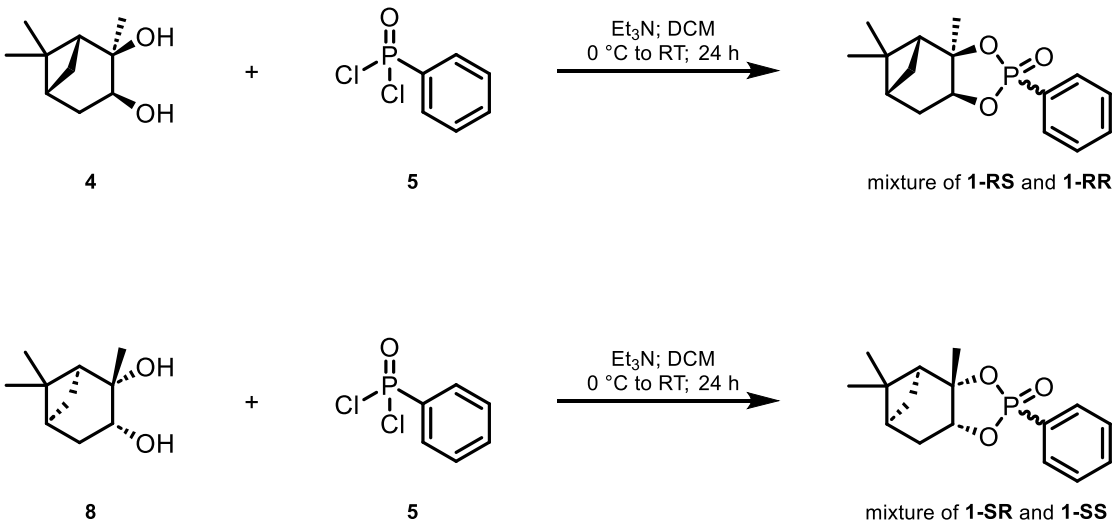
1. Synthesis

1.1. Chemicals and methods

Chemicals were purchased from Sigma Aldrich or Fluorochem/Doug Discovery and used without any further purification. Dry dichloromethane (DCM) was prepared by refluxing DCM with P_2O_5, followed by distillation, and storage over 3 Å molecular sieves. Thin layer chromatography (TLC) was run on silica gel 60 F254 plates (Merck) and compounds/spots were observed under UV light (254 nm). Column chromatography purifications were carried out using VWR International Silica gel 60 (particle size 40–63 µm). Reverse-phase flash column chromatography was carried out using C18 RediSep Rf columns. UPLC samples were measured on Waters UPLC H-Class Core System (column Waters Acquity UPLC BEH C18 1.7 µm, 2.1 mm × 100 mm), Waters Acquity UPLC PDA detector, mass spectrometer Waters SQ D2, and MassLynx mass spectrometry software.

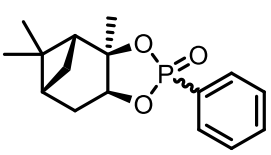
NMR spectra were recorded on Bruker Avance III spectrometer equipped with a broad-band PRODIGY cryo-probe with ATM module (5 mm CPBBO BB-^{1}H/^{19}F/D Z-GRD) operating at 400 MHz for ^{1}H and 100 MHz for ^{13}C. The RDC experiments were performed on Bruker Avance III HD spectrometer with inverse triple resonance cryo-probe and ATM module (5 mm CPTCI ^{1}H/^{13}C/^{15}N/D Z-GRD) operating at 600 MHz for ^{1}H and 151 MHz for ^{13}C. For spectrometer operation and data interpretation, Topspin 3.6 software was used. High-resolution ESI spectra were recorded using an LTQ XL Orbitrap XL (Thermo Fisher Scientific). Optical rotations were measured using AUTOPOL IV (Rudolph Research Analytical, USA).

1.2. Synthetic procedures



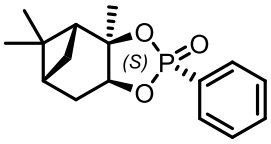
Synthesis was based on a published procedure.[1] A diol of choice (**4** or **8**; *500 mg; 2.9 mmol; 1 eq.*) was dissolved in dry DCM (*30 ml; 0.1M solution of diol*) at 0 °C under an argon atmosphere. To the solution was added Et_3N (*900 µL; 6.46 mmol; 2.2 eq.*) followed by dropwise addition of **5** (*510 µL of 90 % technical grade; 3.2 mmol; 1.1 eq.*). The reaction mixture was stirred at 0 °C for an hour and then at room temperature for an additional 23 h. The excess of **5** was quenched by MeOH, and the reaction mixture was evaporated, adsorbed on silica gel, and purified using reverse phase chromatography (*H_2O/MeCN gradient 5 to 60 % of MeCN*) to afford a mixture of diastereomers. The diastereomers were then separated using column chromatography (*SiO_2; toluene/EtOAc 6:4*) to afford colorless oils, which subsequently solidified.

(3a*R*,4*R*,6*R*,7a*S*)-3a,5,5-trimethyl-2-phenylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaphosphole 2-oxide (mixture of **1-RS** and **1-RR**):



Mixture of **1-RS** and **1-RR** was isolated as a slightly yellow oil (*552 mg; 64 % yield starting from 500 mg of diol*) containing two diastereomers according to NMR. **HR-MS** (ESI) calculated for $C_{16}H_{22}O_3P$, $[M + H]^+$ m/z: 293.13011, found 293.13032.

(2*S*,3a*R*,4*R*,6*R*,7a*S*)-3a,5,5-trimethyl-2-phenylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaphosphole 2-oxide (**1-RS**):



Compound **1-RS** was isolated as white solid (190 mg, *22 % overall yield*), and crystallized from *n*-pentane/EtOAc.

^{1}H NMR (400 MHz, $CDCl_3$, 25°C): δ = 7.83 (m, 2H, 2'), 7.56 (m, 1H, 4'), 7.47 (m, 2H, 3'), 4.67 (ddd, 1H, $J_{6\text{-}5b}$ = 2.6, $J_{6\text{-}5a}$ = 8.9, $J_{6\text{-}P}$ = 13.8, 6), 2.51 (m, 1H, 5a), 2.41 (m, 1H, 7a), 2.31 (dm, 1H, J_{Gem} = 14.8, 5b), 2.25 (m, 1H,2), 2.05 (m, 1H, 4), 2.01 (d, 1H, J_{Gem} = 11.5, 7b), 1.50 (s, 3H, 8), 1.35 (s, 3H, 3-**$CH_{3,a}$**), 0.88 (s, 3H, 3-**$CH_{3,b}$**) ppm.

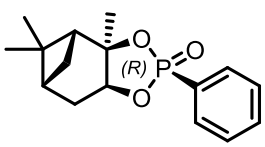
^{13}C NMR (100 MHz, $CDCl_3$, 25°C): δ = 132.65 (d, $J_{4'-P}$ = 3.7, 4´), 131.75 (d, $J_{2'-P}$ = 11.0, 2´), 128.96 (d, $J_{1'-P}$ = 185.8, 1´), 128.72 (d, $J_{3'-P}$ = 15.7, 3´), 90.32 (d, J_{1-P} = 1.5, 1), 80.15 (6), 51.97 (d, J_{2-P} = 4.0, 2), 39.76 (4), 38.61 (3), 35.43 (d, J_{5-P} = 1.8, 5), 28.55 (d, J_{8-P} = 2.6, 8), 27.20 (3-**$CH_{3,a}$**), 26.93 (7), 24.34 (3-**$CH_{3,b}$**) ppm.

^{31}P NMR (161 MHz, $CDCl_3$, 25°C): δ = 37.35 ppm.

HR-MS (ESI) calculated for $C_{16}H_{22}O_3P$, $[M+H]^+$ m/z: 293.13011, found $[M+H]^+$ 293.13016.

$[\alpha]_D^{20}$ −24.8 (*c* 0.270, $CHCl_3$); **R_f:** 0.53 (*toluene/EtOAc 6:4*)

(2*R*,3a*R*,4*R*,6*R*,7a*S*)-3a,5,5-trimethyl-2-phenylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaphosphole 2-oxide (**1-RR**):



Compound **1-RR** was isolated as white solid (145 mg, *17 % overall yield*), and crystallized from *n*-pentane/EtOAc.

^{1}H NMR (600 MHz, $CDCl_3$, 25°C): δ = 7.89 (m, 2H, 2'), 7.57 (m, 1H, 4'), 7.48 (m, 2H, 3'), 4.89 (ddm, 1H, $J_{6\text{-}5b}$ = 2.7, , $J_{6\text{-}P}$ = 6.5, 6), 2.55 (m, 1H, 5a), 2.23−2.18 (m, 2H, 2, 7a), 2.09 (dm, 1H, J_{Gem} = 14.9, 5b), 1.99 (m, 1H, 4), 1.78 (d, 3H, J_{8-P} = 0.5, 8), 1.33−1.24 (m, 4H, 3-**$CH_{3,a}$**, 7b), 0.92 (s, 3H, 3-**$CH_{3,b}$**) ppm.

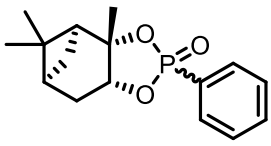
^{13}C NMR (151 MHz, $CDCl_3$, 25°C): δ = 132.88 (d, $J_{4'-P}$ = 3.2, 4´), 132.20 (d, $J_{2'-P}$ = 10.5, 2´), 128.69 (d, $J_{3'-P}$ = 15.5, 3´), 127.10 (d, $J_{1'-P}$ = 186.8, 1´), 90.10 (d, J_{1-P} = 1.4, 1), 79.56 (d, J_{6-P} = 1.6, 6), 51.86 (d, J_{2-P} = 7.4, 2), 39.68 (4), 38.87 (3), 35.14 (d, J_{5-P} = 4.8, 5), 29.40 (8), 27.16 (3-**$CH_{3,a}$**), 26.88 (7), 24.34 (3-**$CH_{3,b}$**) ppm.

^{31}P NMR (161 MHz, $CDCl_3$, 25°C): δ = 37.12 ppm.

HR-MS (ESI) Calculated for $C_{16}H_{22}O_3P$, $[M+H]^+$ m/z: 293.13011, $[M+H]^+$, found 293.13015.

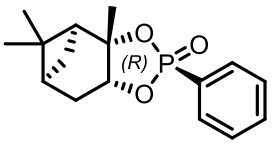
$[\alpha]_D^{20}$ 0 (*c* 0.280, $CHCl_3$); **R_f:** 0.35 (*toluene/EtOAc 6:4*)

(3a*S*,4*S*,6*S*,7a*R*)-3a,5,5-trimethyl-2-phenylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaphosphole 2-oxide (mixture of **1-SR** and **1-SS**):



Mixture of **1-SR** and **1-SS** was isolated as a slightly yellow oil (*561 mg, 65 % yield starting from 500 mg of diol*) containing two diastereomers according to NMR. **HR-MS** (ESI) calculated for $C_{16}H_{22}O_3P$,$[M + H]^+$ m/z: 293.13011, $[M + H]^+$, found 293.13000.

(2*R*,3a*S*,4*S*,6*S*,7a*R*)-3a,5,5-trimethyl-2-phenylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaphosphole 2-oxide (**1-SR**):



Compound **1-SR** was isolated as a white solid (400 mg, 47 *% overall yield*), and crystallized from *n*-pentane/EtOAc.

^{1}H NMR (400 MHz, $CDCl_3$, 25°C): δ = 7.83 (m, 2H, 2'), 7.56 (m, 1H, 4'), 7.47 (m, 2H, 3'), 4.67 (ddd, 1H, $J_{6\text{-}5b}$ = 2.6, $J_{6\text{-}5a}$ = 8.9, $J_{6\text{-}P}$ = 13.8, 6), 2.51 (m, 1H, 5a), 2.41 (m, 1H, 7a), 2.31 (dm, 1H, J_{Gem} = 14.8, 5b), 2.25 (m, 1H, 2), 2.05 (m, 1H, 4), 2.01 (d, 1H, J_{Gem} = 11.5, 7b), 1.50 (s, 3H, 8), 1.35 (s, 3H, 3-**$CH_{3,a}$**), 0.88 (s, 3H, 3-**$CH_{3,b}$**) ppm**.**

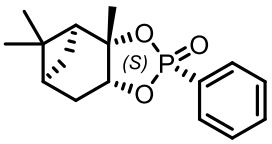
^{13}C NMR (100 MHz, $CDCl_3$, 25°C): δ = 132.65 (d, $J_{4'-P}$ = 3.7, 4´), 131.75 (d, $J_{2'-P}$ = 11.0, 2´), 128.96 (d, $J_{1'-P}$ = 185.8, 1´), 128.72 (d, $J_{3'-P}$ = 15.7, 3´), 90.32 (d, J_{1-P} = 1.5, 1), 80.15 (d, J_{6-P} = 1.0, 6), 51.97 (d, J_{2-P} = 4.0, 2), 39.76 (4), 38.61 (3), 35.43 (d, J_{5-P} = 1.8, 5), 28.55 (d, J_{8-P} = 2.6, 8), 27.20 (3-**$CH_{3,a}$**), 26.93 (7), 24.34 (3-**$CH_{3,b}$**) ppm.

^{31}P NMR (161 MHz, $CDCl_3$, 25°C): δ = 37.34 ppm.

HR-MS (ESI) calculated for $C_{16}H_{22}O_3P$, $[M+H]^+$ m/z: 293.13011, found $[M+H]^+$ 293.13023.

$[\alpha]_D^{20}$ 30.0 (*c* 0.583, $CHCl_3$); **R_f:** 0.53 (*toluene/EtOAc 6:4*)

(2*S*,3a*S*,4*S*,6*S*,7a*R*)-3a,5,5-trimethyl-2-phenylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaphosphole 2-oxide (**1-SS**):



Compound **1-SS** was isolated as a white solid (101 mg, *12 % overall yield*), and crystallized from *n*-pentane/EtOAc.

^{1}H NMR (400 MHz, $CDCl_3$, 25°C): δ = 7.89 (m, 2H, 2'), 7.57 (m, 1H, 4'), 7.48 (m, 2H, 3'), 4.89 (ddm, 1H, $J_{6\text{-}5b}$ = 2.7, , $J_{6\text{-}P}$ = 6.5, 6), 2.55 (m, 1H, 5a), 2.25−2.17 (m, 2H, 2, 7a), 2.09 (dm, 1H, J_{Gem} = 14.9, 5b), 1.99 (m, 1H, 4), 1.78 (s, 3H, 8), 1.33−1.24 (m, 4H, 3-**$CH_{3,a}$**, 7b), 0.92 (s, 3H, 3-**$CH_{3,b}$**) ppm.

^{13}C NMR (100 MHz, $CDCl_3$, 25°C): δ = 132.88 (d, $J_{4'-P}$ = 3.2, 4´), 132.20 (d, $J_{2'-P}$ = 10.3, 2´), 128.69 (d, $J_{3'-P}$ = 15.7, 3´), 127.10 (d, $J_{1'-P}$ = 186.6, 1´), 90.10 (1), 79.56 (d, J_{6-P} = 1.6, 6), 51.86 (d, J_{2-P} = 7.3, 2), 39.68 (4), 38.87 (3), 35.14 (d, J_{5-P} = 5.0, 5), 29.40 (8), 27.16 (3-**$CH_{3,a}$**), 26.88 (7), 24.34 (3-**$CH_{3,b}$**) ppm.

^{31}P NMR (161 MHz, $CDCl_3$, 25°C): δ = 37.12 ppm.

HR-MS (ESI) calculated for $C_{16}H_{22}O_3P$, $[M+H]^+$ m/z: 293.13011, found $[M+H]^+$ 293.12960.

$[\alpha]_D^{20}$ 0 (*c* 0.256, $CHCl_3$); **R_f:** 0.35 (*toluene/EtOAc 6:4*)

2. Samples composition

Table S1: Composition of individual samples prepared for RDC measurements.

Compound	m (compound) [mg]	m ($CDCl_3$) [mg]	m (PBLG) [mg]	w (medium) [%]
1-RS	5.1	900.0	77.3	7.9
1-RR	5.0	900.0	77.4	7.9
1-SR	5.1	900.0	77.6	7.9
1-SS	5.0	900.0	77.6	7.9
2-SR	5.0	900.0	65.2	6.7
2-RR	5.1	900.0	77.3	7.9
3-A	5.0	1177.5	77.3	6.1
3-B	5.0	900.0	77.3	7.9

3. Computational part

3.1. Results of P3D/PALES simulations and relative energies of individual conformers

All computations were done as described in the Experimental section of the main text.

Table S2: Energies of conformers of isomers of **1** obtained from docking relative to the energy of global minimum (GM; $\Delta E = E(\text{conf.}) - E(\text{GM})$, where E is the electronic energy of the given system).

Isomer	Conformer	ΔE (kcal mol^{-1})	R (**1-SR** data)	R (**1-SS** data)	R (**1-RS** data)	R (**1-RR** data)
1-SR	GM	0.0	0.925	0.617	0.931	0.603
1-SR	A	5.9	0.904	0.590	0.906	0.581
1-SR	B	6.0	0.881	0.577	0.876	0.566
1-SR	C	6.0	0.892	0.603	0.885	0.591
1-SR	D	6.0	0.914	0.616	0.914	0.606
1-SS	GM	0.0	0.970	0.815	0.983	0.763
1-SS	A	5.6	0.962	0.827	0.976	0.779
1-RS	GM	0.0	0.925	0.616	0.930	0.602
1-RS	A	13.4	0.900	0.607	0.897	0.597
1-RS	B	13.6	0.915	0.619	0.918	0.611
1-RS	C	15.2	0.899	0.634	0.889	0.620
1-RR	GM	0.0	0.970	0.812	0.983	0.759
1-RR	A	13.2	0.934	0.851	0.948	0.811
1-RR	B	13.7	0.959	0.824	0.973	0.777
1-RR	C	13.7	0.961	0.839	0.974	0.790

Table S3: Energies of conformers of isomers of **1** obtained from docking and optimized by normal mode relaxation relative to the energy of global minimum (GM; $\Delta E = E(\text{conf.}) - E(\text{GM})$, where E is the electronic energy of the given system).

Isomer	Conformer	ΔE (kcal mol^{-1})	R (**1-SR** data)	R (**1-SS** data)	R (**1-RS** data)	R (**1-RR** data)
1-SR	D	1.1	0.920	0.611	0.920	0.592
1-SR	A	1.1	0.912	0.590	0.914	0.573
1-SR	B	1.3	0.890	0.574	0.884	0.555
1-SR	C	1.3	0.899	0.597	0.891	0.576
1-SS	A	1.0	0.959	0.809	0.975	0.756
1-RS	B	2.4	0.922	0.615	0.924	0.599
1-RS	A	2.7	0.908	0.603	0.905	0.585
1-RS	C	4.2	0.905	0.625	0.896	0.606
1-RR	A	2.4	0.933	0.823	0.951	0.775
1-RR	C	2.6	0.959	0.821	0.974	0.768
1-RR	B	2.9	0.956	0.806	0.972	0.753

Table S4: Energies of conformers of isomers of **2** obtained from docking relative to the energy of global minimum (GM; $\Delta E = E(\text{conf.}) - E(\text{GM})$, where E is the electronic energy of the given system).

Isomer	Conformer	ΔE (kcal mol^{-1})	R (**2-SR** data)	R (**2-RR** data)
2-SR	A	4.1	0.850	0.544
2-SR	B	4.6	0.827	0.509
2-SR	C	4.7	0.725	0.365
2-SR	D	5.1	0.728	0.366
2-SR	E	5.1	0.914	0.654
2-SR	F	5.2	0.925	0.675
2-SR	G	5.4	0.849	0.542
2-SR	H	5.5	0.618	0.224
2-SR	I	5.6	0.987	0.827
2-SR	J	5.7	0.552	0.146
2-SR	K	6.1	0.755	0.404
2-SR	L	6.2	0.446	0.025
2-SR	M	6.4	0.426	0.003
2-SR	N	6.4	0.969	0.772
2-SR	O	6.8	0.351	0.076
2-SR	P	7.3	0.765	0.413
2-SR	Q	7.4	0.965	0.837
2-SR	R	8.0	0.994	0.857
2-SR	S	8.2	0.973	0.782
2-SR	T	8.6	0.337	0.039
2-SR	U	9.9	0.566	0.164
2-RR	A	4.0	0.984	0.965
2-RR	B	4.0	0.973	0.978
2-RR	C	4.3	0.974	0.977
2-RR	D	4.4	0.975	0.976
2-RR	E	4.5	0.982	0.968
2-RR	F	4.5	0.995	0.936
2-RR	G	4.7	0.995	0.941
2-RR	H	4.8	0.974	0.978
2-RR	I	4.8	0.995	0.941
2-RR	J	4.9	0.927	0.678
2-RR	K	4.9	0.977	0.795
2-RR	L	5.0	0.974	0.977
2-RR	M	5.1	0.990	0.953
2-RR	N	5.1	0.990	0.954
2-RR	O	5.4	0.974	0.978
2-RR	P	5.6	0.983	0.967
2-RR	Q	7.1	0.996	0.867
2-RR	R	7.4	0.981	0.970
2-RR	S	8.4	0.979	0.973
2-RR	T	8.4	0.998	0.884
2-RR	U	8.5	0.967	0.767

Table S5: Energies of conformers of isomers of **2** obtained from docking and optimized by normal mode relaxation relative to the energy of global minimum (GM; ΔE = E(conf.) – E(GM), where E is the electronic energy of the given system).

Isomer	Conformer	ΔE (kcal mol^{-1})	R (**2-SR** data)	R (**2-RR** data)
2-SR	A	1.3	0.920	0.665
2-SR	C	1.8	0.823	0.502
2-SR	B	2.2	0.877	0.588
2-SR	D	2.3	0.822	0.499
2-SR	H	2.5	0.626	0.233
2-SR	F	2.6	0.970	0.775
2-SR	E	2.8	0.964	0.761
2-SR	G	2.8	0.840	0.529
2-SR	J	3.1	0.577	0.174
2-SR	I	3.2	0.993	0.853
2-SR	K	3.3	0.858	0.557
2-SR	L	3.7	0.456	0.037
2-SR	M	3.8	0.443	0.022
2-SR	U	3.9	0.736	0.379
2-SR	N	4.0	0.966	0.764
2-SR	O	4.2	0.399	0.026
2-SR	P	4.5	0.851	0.543
2-SR	Q	5.0	0.992	0.846
2-SR	R	5.6	0.999	0.915
2-SR	S	5.8	0.996	0.868
2-SR	T	6.1	0.380	0.045
2-RR	B	1.5	0.971	0.979
2-RR	E	1.7	0.981	0.968
2-RR	A	1.7	0.977	0.973
2-RR	D	1.8	0.975	0.975
2-RR	G	1.9	0.995	0.939
2-RR	F	2.0	0.999	0.914
2-RR	C	2.0	0.972	0.978
2-RR	H	2.2	0.972	0.978
2-RR	I	2.3	0.995	0.941
2-RR	L	2.3	0.973	0.978
2-RR	M	2.6	0.989	0.955
2-RR	N	2.6	0.989	0.956
2-RR	O	2.8	0.972	0.978
2-RR	J	2.9	0.925	0.679
2-RR	K	3.0	0.933	0.695
2-RR	P	3.2	0.990	0.954
2-RR	R	4.7	0.980	0.970
2-RR	Q	4.9	0.976	0.793
2-RR	S	5.7	0.990	0.955
2-RR	T	5.8	0.998	0.883
2-RR	U	6.1	0.998	0.877

Table S6: Energies of conformers of isomers of **3** obtained from docking relative to the energy of global minimum (GM; $\Delta E = E(\text{conf.}) - E(\text{GM})$, where E is the electronic energy of the given system).

Isomer	Conformer	ΔE (kcal mol^{-1})	R (**3-A** data)	R (**3-B** data)
3-RR	A	6.2	0.306	0.385
3-RR	B	6.7	0.434	0.204
3-RR	C	7.1	0.403	0.227
3-RR	D	7.2	0.228	0.381
3-RR	E	7.3	0.446	0.227
3-RR	F	7.5	0.507	0.094
3-RR	G	7.6	0.540	0.107
3-RR	H	8.1	0.280	0.055
3-RR	I	8.1	0.570	0.035
3-RR	J	8.3	0.438	0.246
3-RR	K	8.5	0.266	0.406
3-RR	L	8.6	0.171	0.422
3-RR	M	8.6	0.220	0.498
3-RR	N	8.9	0.131	0.224
3-RR	O	9.0	0.125	0.218
3-RR	P	9.0	0.074	0.477
3-RR	Q	9.0	0.074	0.498
3-RR	R	9.1	0.006	0.616
3-RR	S	9.2	0.612	0.025
3-RR	T	9.3	0.644	0.110
3-RR	U	9.7	0.328	0.399
3-RR	V	9.9	0.821	0.297
3-RR	W	10.0	0.466	0.200
3-RR	X	10.0	0.246	0.002
3-RR	Y	10.1	0.684	0.260
3-RR	Z	10.3	0.130	0.166
3-RR	AA	10.7	0.811	0.298
3-RR	AB	10.8	0.454	0.210
3-RR	AC	11.0	0.167	0.119
3-RR	AD	11.1	0.587	0.153
3-RR	AE	11.1	0.470	0.221
3-RR	AF	11.1	0.357	0.370
3-RR	AG	11.2	0.405	0.260
3-RR	AH	11.2	0.123	0.173
3-RS	A	6.1	0.630	0.376
3-RS	B	6.3	0.605	0.318
3-RS	C	6.4	0.642	0.406
3-RS	D	6.5	0.695	0.495
3-RS	E	6.6	0.716	0.511
3-RS	F	6.6	0.708	0.509
3-RS	G	6.6	0.681	0.495
3-RS	H	6.8	0.714	0.490
3-RS	I	6.8	0.688	0.456
3-RS	J	7.9	0.702	0.024

3-RS	K	8.1	0.359	0.077
3-RS	L	8.2	0.456	0.087
3-RS	M	8.7	0.914	0.469
3-RS	N	9.5	0.562	0.184
3-RS	O	11.8	0.407	0.359
3-RS	P	11.8	0.446	0.263
3-RS	Q	11.8	0.130	0.350
3-RS	R	11.9	0.041	0.415
3-RS	S	12.1	0.082	0.440
3-RS	T	12.5	0.008	0.472
3-RS	U	13.9	0.472	0.193
3-RS	V	14.2	0.650	0.058
3-RS	W	14.2	0.248	0.435

Table S7: Energies of conformers of isomers of **3** obtained from docking and optimized by normal mode relaxation relative to the energy of global minimum (GM; $\Delta E = E(\text{conf.}) - E(\text{GM})$, where E is the electronic energy of the given system).

Isomer	Conformer	ΔE (kcal mol^{-1})	R (**3-A** data)	R (**3-B** data)
3-RR	A	2.6	0.386	0.328
3-RR	B	3.2	0.541	0.071
3-RR	E	3.7	0.486	0.106
3-RR	F	3.9	0.540	0.043
3-RR	D	3.9	0.341	0.285
3-RR	C	3.9	0.566	0.058
3-RR	G	4.3	0.573	0.050
3-RR	I	4.6	0.557	0.087
3-RR	H	4.7	0.427	0.128
3-RR	L	5.0	0.208	0.462
3-RR	K	5.0	0.345	0.387
3-RR	J	5.1	0.498	0.201
3-RR	M	5.3	0.359	0.358
3-RR	N	5.5	0.198	0.170
3-RR	Q	5.6	0.179	0.197
3-RR	O	5.7	0.182	0.175
3-RR	P	5.8	0.168	0.432
3-RR	S	5.9	0.631	0.002
3-RR	R	6.1	0.005	0.622
3-RR	T	6.2	0.630	0.096
3-RR	V	6.3	0.827	0.285
3-RR	Y	6.4	0.682	0.278
3-RR	X	6.5	0.240	0.004
3-RR	Z	6.7	0.125	0.164
3-RR	W	6.7	0.486	0.216
3-RR	AA	6.8	0.795	0.272
3-RR	U	6.9	0.316	0.407
3-RR	AD	7.0	0.559	0.172
3-RR	AB	7.4	0.486	0.189

3-RR	AE	7.6	0.487	0.215
3-RR	AH	7.8	0.122	0.174
3-RR	AC	7.8	0.162	0.122
3-RR	AF	8.1	0.356	0.373
3-RR	AG	8.4	0.394	0.268
3-RS	A	2.0	0.801	0.601
3-RS	B	2.2	0.788	0.555
3-RS	G	2.9	0.803	0.606
3-RS	D	3.0	0.791	0.609
3-RS	C	3.0	0.757	0.528
3-RS	E	3.2	0.811	0.631
3-RS	F	3.2	0.812	0.625
3-RS	H	3.2	0.809	0.630
3-RS	I	3.2	0.819	0.601
3-RS	J	3.9	0.695	0.059
3-RS	K	4.7	0.608	0.244
3-RS	L	4.8	0.704	0.405
3-RS	M	5.3	0.956	0.580
3-RS	N	5.4	0.571	0.167
3-RS	Q	7.7	0.301	0.219
3-RS	R	7.8	0.191	0.294
3-RS	S	8.1	0.223	0.335
3-RS	O	8.3	0.433	0.361
3-RS	P	8.4	0.628	0.007
3-RS	T	8.5	0.145	0.346
3-RS	V	10.7	0.693	0.043
3-RS	U	10.7	0.519	0.207
3-RS	W	11.0	0.318	0.423

3.2. Detailed P3D/PALES results

All RDC values are given in Hz. The atom numbering used in the tables corresponds to the numbering in Figure 1 of the main text.

Table S8: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs								
		GM	Unrelaxed				Relaxed			
			A	B	C	D	A	B	C	D
C4'-H4'	-13.11	-27.23	-28.67	-28.90	-27.66	-27.41	-28.22	-28.60	-27.48	-27.19
C2-H2	31.36	23.40	21.37	19.56	20.32	22.10	21.82	19.90	20.51	22.36
C4-H4	0.40	-7.11	-8.31	-9.45	-9.78	-8.62	-6.87	-7.91	-8.21	-7.12
C6-H6	15.42	12.31	14.77	18.43	18.31	14.67	14.67	18.35	18.28	14.79
C1-C8	-0.57	1.13	0.99	1.07	1.04	0.99	1.00	1.10	1.07	1.01
C4'-P	-0.04	-0.14	-0.14	-0.15	-0.14	-0.14	-0.15	-0.15	-0.15	-0.15
C1'-P	-1.21	-2.37	-2.37	-2.42	-2.38	-2.38	-2.42	-2.47	-2.43	-2.41
C1-P	1.28	-0.57	-0.62	-0.65	-0.65	-0.61	-0.61	-0.64	-0.64	-0.60
C6-P	0.70	-0.51	-0.42	-0.40	-0.38	-0.41	-0.44	-0.42	-0.40	-0.42
C8-P	-0.38	-0.01	-0.03	-0.03	-0.03	-0.03	-0.03	-0.03	-0.03	-0.03
R		0.925	0.904	0.881	0.892	0.914	0.912	0.890	0.899	0.920

Table S9: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs								
		GM	Unrelaxed				Relaxed			
			A	B	C	D	A	B	C	D
C4'-H4'	7.03	-43.91	-47.14	-47.31	-43.82	-43.62	-46.84	-47.67	-44.56	-43.89
C2-H2	35.55	37.73	35.13	32.01	32.19	35.17	36.22	33.17	33.26	36.09
C4-H4	-11.31	-11.47	-13.66	-15.46	-15.50	-13.72	-11.41	-13.19	-13.32	-11.50
C6-H6	15.88	19.85	24.28	30.17	29.00	23.36	24.34	30.58	29.63	23.88
C1-C8	-1.96	1.82	1.63	1.75	1.65	1.58	1.66	1.83	1.74	1.63
C4'-P	-0.25	-0.23	-0.24	-0.24	-0.23	-0.23	-0.24	-0.25	-0.24	-0.23
C1'-P	0.41	-3.83	-3.90	-3.95	-3.77	-3.78	-4.02	-4.12	-3.95	-3.89
C1-P	1.30	-0.92	-1.01	-1.06	-1.03	-0.97	-1.01	-1.06	-1.04	-0.97
C6-P	0.66	-0.82	-0.69	-0.66	-0.61	-0.66	-0.73	-0.70	-0.65	-0.68
C5-P	-0.39	-0.44	-0.44	-0.46	-0.43	-0.41	-0.45	-0.47	-0.44	-0.41
R		0.617	0.590	0.577	0.603	0.616	0.590	0.574	0.597	0.611

Table S10: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs								
		GM	Unrelaxed				Relaxed			
			A	B	C	D	A	B	C	D
C4'-H4'	-17.64	-33.13	-34.99	-35.56	-34.10	-33.55	-34.51	-35.26	-33.96	-33.32
C2-H2	39.33	28.47	26.07	24.06	25.05	27.05	26.69	24.53	25.35	27.40
C4-H4	1.26	-8.65	-10.14	-11.62	-12.06	-10.55	-8.41	-9.75	-10.15	-8.73
C6-H6	15.89	14.98	18.02	22.68	22.57	17.97	17.93	22.62	22.58	18.13
C1-C8	-0.8	1.38	1.21	1.31	1.28	1.21	1.22	1.35	1.32	1.24
C4'-P	-0.34	-0.18	-0.18	-0.18	-0.18	-0.17	-0.18	-0.18	-0.18	-0.18
C8-P	-0.63	-0.02	-0.04	-0.03	-0.04	-0.04	-0.04	-0.04	-0.04	-0.04
R		0.931	0.906	0.876	0.885	0.914	0.914	0.884	0.891	0.920

Table S2: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs								
		GM	Unrelaxed				Relaxed			
			A	B	C	D	A	B	C	D
C4'-H4'	7.99	-42.05	-44.88	-45.29	-41.99	-41.65	-45.27	-46.24	-43.25	-42.55
C2-H2	34.54	36.13	33.45	30.64	30.84	33.59	35.01	32.17	32.28	34.99
C4-H4	-13.18	-10.98	-13.01	-14.80	-14.85	-13.10	-11.03	-12.79	-12.92	-11.15
C6-H6	14.43	19.01	23.12	28.88	27.79	22.30	23.53	29.66	28.76	23.16
C1-C8	-2.15	1.75	1.55	1.67	1.58	1.50	1.60	1.77	1.68	1.58
R		0.603	0.581	0.566	0.591	0.606	0.573	0.555	0.576	0.592

Table S12: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs		
		GM	Unrelaxed	Relaxed
C4'-H4'	-13.11	-11.36	-10.65	-10.66
C2-H2	31.36	35.42	36.13	36.45
C4-H4	0.40	0.61	-0.18	1.56
C6-H6	15.42	8.23	7.41	7.11
C1-C8	-0.57	0.73	0.69	0.70
C4'-P	-0.04	-0.06	-0.05	-0.05
C1'-P	-1.21	-0.92	-0.78	-0.80
C1-P	1.28	-1.27	-1.38	-1.33
C6-P	0.70	-0.96	-0.94	-0.92
C8-P	-0.38	-0.37	-0.39	-0.39
R		0.970	0.962	0.959

Table S33: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs		
		GM	Unrelaxed	Relaxed
C4'-H4'	7.03	-14.50	-13.33	-13.55
C2-H2	35.55	45.22	45.19	46.31
C4-H4	-11.31	0.77	-0.23	1.98
C6-H6	15.88	10.51	9.27	9.03
C1-C8	-1.96	0.93	0.87	0.89
C4'-P	-0.25	-0.07	-0.07	-0.07
C1'-P	0.41	-1.17	-0.98	-1.02
C1-P	1.30	-1.62	-1.73	-1.69
C6-P	0.66	-1.23	-1.17	-1.18
C5-P	-0.39	-0.29	-0.27	-0.28
R		0.815	0.827	0.809

Table S14: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs		
		GM	Unrelaxed	Relaxed
C4'-H4'	-17.64	-14.03	-13.14	-13.17
C2-H2	39.33	43.77	44.56	45.01
C4-H4	1.26	0.75	-0.22	1.93
C6-H6	15.89	10.17	9.14	8.78
C1-C8	-0.8	0.90	0.86	0.86
C4'-P	-0.34	-0.07	-0.06	-0.07
C8-P	-0.63	-0.46	-0.48	-0.48
R		0.983	0.976	0.975

Table S15: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs		
		GM	Unrelaxed	Relaxed
C4'-H4'	7.99	-15.29	-13.92	-14.38
C2-H2	34.54	47.68	47.19	49.15
C4-H4	-13.18	0.82	-0.24	2.11
C6-H6	14.43	11.08	9.68	9.58
C1-C8	-2.15	0.98	0.91	0.94
R		0.763	0.779	0.756

Table S16: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	-13.11	-27.25	-27.76	-27.46	-26.08	-27.49	-27.18	-26.21
C2-H2	31.36	23.31	20.97	22.43	20.93	21.29	22.72	21.11
C4-H4	0.40	-7.12	-9.43	-8.72	-10.49	-7.88	-7.31	-9.11
C6-H6	15.42	12.52	16.67	13.80	18.79	16.69	13.84	18.50
C1-C8	-0.57	1.15	0.98	1.01	1.03	1.00	1.02	1.04
C4'-P	-0.04	-0.14	-0.14	-0.14	-0.14	-0.14	-0.14	-0.14
C1'-P	-1.21	-2.37	-2.33	-2.33	-2.29	-2.37	-2.36	-2.33
C1-P	1.28	-0.57	-0.63	-0.61	-0.66	-0.63	-0.59	-0.65
C6-P	0.70	-0.52	-0.36	-0.45	-0.34	-0.37	-0.46	-0.36
C8-P	-0.38	-0.01	-0.03	-0.02	-0.03	-0.03	-0.03	-0.03
R		0.925	0.900	0.915	0.899	0.908	0.922	0.905

Table S17: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	7.03	-43.90	-44.26	-43.66	-39.69	-44.48	-43.79	-40.74
C2-H2	35.55	37.55	33.44	35.66	31.85	34.45	36.59	32.81
C4-H4	-11.31	-11.47	-15.03	-13.87	-15.97	-12.75	-11.78	-14.16
C6-H6	15.88	20.17	26.58	21.95	28.59	27.01	22.29	28.75
C1-C8	-1.96	1.86	1.56	1.61	1.56	1.62	1.64	1.61
C4'-P	-0.25	-0.23	-0.23	-0.22	-0.21	-0.23	-0.23	-0.22
C1'-P	0.41	-3.82	-3.71	-3.71	-3.48	-3.84	-3.80	-3.62
C1-P	1.30	-0.92	-1.01	-0.96	-1.01	-1.02	-0.96	-1.01
C6-P	0.66	-0.84	-0.57	-0.72	-0.52	-0.60	-0.74	-0.56
C5-P	-0.39	-0.44	-0.38	-0.43	-0.37	-0.39	-0.43	-0.38
R		0.616	0.607	0.619	0.634	0.603	0.615	0.625

Table S18: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	-17.64	-33.17	-34.08	-33.54	-32.34	-33.83	-33.22	-32.51
C2-H2	39.33	28.38	25.75	27.39	25.95	26.20	27.76	26.18
C4-H4	1.26	-8.67	-11.57	-10.65	-13.01	-9.69	-8.94	-11.30
C6-H6	15.89	15.24	20.47	16.86	23.29	20.54	16.91	22.95
C1-C8	-0.8	1.41	1.20	1.23	1.27	1.23	1.25	1.29
C4'-P	-0.34	-0.18	-0.17	-0.17	-0.17	-0.18	-0.17	-0.17
C8-P	-0.63	-0.02	-0.04	-0.03	-0.03	-0.04	-0.03	-0.04
R		0.930	0.897	0.918	0.889	0.905	0.924	0.896

Table S19: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	7.99	-42.13	-42.24	-41.48	-38.13	-43.10	-42.23	-39.55
C2-H2	34.54	36.04	31.91	33.88	30.60	33.38	35.29	31.85
C4-H4	-13.18	-11.01	-14.34	-13.17	-15.34	-12.35	-11.36	-13.75
C6-H6	14.43	19.36	25.36	20.85	27.47	26.17	21.50	27.91
C1-C8	-2.15	1.78	1.49	1.53	1.50	1.56	1.58	1.57
R		0.602	0.597	0.611	0.620	0.585	0.599	0.606

Table S20: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	-13.11	-11.45	-7.94	-10.59	-9.30	-8.23	-10.48	-9.59
C2-H2	31.36	35.37	38.37	36.31	36.65	38.56	36.62	36.78
C4-H4	0.40	0.78	-1.11	-0.02	0.41	1.58	1.83	1.84
C6-H6	15.42	8.17	5.51	6.99	8.13	5.38	6.79	7.83
C1-C8	-0.57	0.74	0.72	0.62	0.61	0.68	0.58	0.59
C4'-P	-0.04	-0.06	-0.04	-0.05	-0.05	-0.04	-0.05	-0.05
C1'-P	-1.21	-0.93	-0.66	-0.77	-0.72	-0.70	-0.79	-0.73
C1-P	1.28	-1.27	-1.36	-1.39	-1.42	-1.30	-1.33	-1.36
C6-P	0.70	-0.97	-0.99	-0.94	-0.95	-0.98	-0.92	-0.93
C8-P	-0.38	-0.38	-0.37	-0.40	-0.41	-0.37	-0.40	-0.41
R		0.970	0.934	0.959	0.961	0.933	0.956	0.959

Table S21: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	7.03	-14.72	-9.36	-13.25	-11.45	-10.04	-13.36	-12.00
C2-H2	35.55	45.46	45.26	45.42	45.10	47.03	46.68	46.05
C4-H4	-11.31	1.00	-1.31	-0.03	0.51	1.93	2.34	2.30
C6-H6	15.88	10.51	6.50	8.74	10.01	6.56	8.65	9.80
C1-C8	-1.96	0.95	0.85	0.78	0.75	0.82	0.74	0.73
C4'-P	-0.25	-0.08	-0.05	-0.06	-0.06	-0.05	-0.07	-0.06
C1'-P	0.41	-1.19	-0.78	-0.96	-0.88	-0.86	-1.01	-0.91
C1-P	1.30	-1.64	-1.61	-1.74	-1.74	-1.59	-1.70	-1.71
C6-P	0.66	-1.24	-1.17	-1.17	-1.17	-1.19	-1.17	-1.17
C5-P	-0.39	-0.29	-0.27	-0.27	-0.28	-0.29	-0.28	-0.29
R		0.812	0.851	0.824	0.839	0.823	0.806	0.821

Table S22: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	-17.64	-14.19	-9.83	-13.06	-11.54	-10.20	-12.98	-11.87
C2-H2	39.33	43.84	47.52	44.78	45.44	47.76	45.35	45.53
C4-H4	1.26	0.96	-1.38	-0.03	0.51	1.96	2.27	2.28
C6-H6	15.89	10.13	6.82	8.62	10.08	6.66	8.41	9.69
C1-C8	-0.8	0.92	0.89	0.77	0.75	0.84	0.72	0.72
C4'-P	-0.34	-0.07	-0.05	-0.06	-0.06	-0.05	-0.06	-0.06
C8-P	-0.63	-0.47	-0.46	-0.50	-0.51	-0.46	-0.50	-0.51
R		0.983	0.948	0.973	0.974	0.951	0.972	0.974

Table S23: Theoretical (calculated) RDCs of the global minimum (GM) and conformers of **1-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs						
		GM	Unrelaxed			Relaxed		
			A	B	C	A	B	C
C4'-H4'	7.99	-15.53	-9.72	-13.85	-12.07	-10.60	-14.19	-12.82
C2-H2	34.54	47.95	46.98	47.46	47.54	49.67	49.59	49.19
C4-H4	-13.18	1.05	-1.36	-0.03	0.54	2.03	2.48	2.46
C6-H6	14.43	11.08	6.74	9.14	10.55	6.93	9.19	10.47
C1-C8	-2.15	1.01	0.88	0.81	0.79	0.87	0.79	0.78
R		0.759	0.811	0.777	0.790	0.775	0.753	0.768

Table S24: Theoretical (calculated) RDCs of conformers of **2-SR** derived from molecular docking; normalized against **2-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**	**K**	**L**	**M**	**N**	**O**
C4'-H4'	-15.10	-20.15	-20.65	-22.73	-22.69	-18.74	-18.49	-20.17	-25.28	-16.46	-27.13	-22.12	-31.02	-31.94	-18.98	-36.30
C2-H2	-9.75	-1.32	-0.53	3.24	3.11	-3.74	-4.22	-1.28	7.71	-7.60	11.00	2.15	17.97	19.57	-3.37	27.09
C4'-P	0.10	-0.10	-0.11	-0.12	-0.11	-0.09	-0.09	-0.11	-0.13	-0.09	-0.14	-0.11	-0.16	-0.16	-0.10	-0.19
C1'-P	-1.54	-1.71	-1.77	-1.92	-1.89	-1.52	-1.54	-1.73	-2.05	-1.42	-2.41	-1.93	-2.63	-2.63	-1.71	-3.15
C1-P	0.46	-0.06	-0.13	-0.18	0.04	-0.02	0.07	-0.11	0.14	0.05	0.07	-0.15	0.16	0.18	-0.06	0.10
C2-P	0.17	-0.18	-0.26	-0.07	-0.31	-0.10	-0.16	-0.22	-0.25	0.05	-0.20	-0.13	-0.01	-0.03	-0.18	-0.04
C5-P	-0.17	-0.04	-0.03	0.01	-0.13	-0.13	-0.18	0.01	0.04	-0.07	0.22	0.00	0.15	0.04	-0.05	0.13
C3-P	-0.01	-0.12	-0.15	-0.11	-0.20	-0.09	-0.11	-0.13	-0.34	-0.02	-0.35	-0.12	-0.33	-0.35	-0.11	-0.46
C4-P	-0.09	-0.17	-0.17	-0.17	-0.12	-0.16	-0.17	-0.05	-0.20	-0.09	-0.18	-0.05	-0.21	-0.22	-0.06	-0.28
R		0.850	0.827	0.725	0.728	0.914	0.925	0.849	0.618	0.987	0.552	0.755	0.446	0.426	0.904	0.351
Q		0.390	0.379	0.427	0.371	0.401	0.378	0.350	0.482	0.416	0.482	0.388	0.552	0.566	0.349	0.576

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	**Q**	**R**	**S**	**T**	**U**
C4'-H4'	-15.10	-21.83	-17.40	-16.02	-17.06	-37.32	-26.77
C2-H2	-9.75	1.84	-6.12	-8.39	-6.56	28.69	10.26
C4'-P	0.10	-0.11	-0.09	-0.08	-0.09	-0.19	-0.14
C1'-P	-1.54	-1.77	-1.55	-1.41	-1.39	-3.15	-2.25
C1-P	0.46	0.48	-0.03	0.01	0.34	-0.11	-0.27
C2-P	0.17	-0.05	-0.12	0.04	0.04	-0.23	-0.14
C5-P	-0.17	-0.39	-0.13	-0.12	-0.38	0.11	-0.12
C3-P	-0.01	-0.14	-0.08	-0.02	-0.06	-0.52	-0.14
C4-P	-0.09	-0.17	-0.06	-0.03	-0.12	-0.31	-0.06
R		0.765	0.965	0.994	0.973	0.337	0.566
Q		0.383	0.368	0.426	0.370	0.575	0.426

Table S25: Theoretical (calculated) RDCs of conformers of **2-SR** derived from molecular docking; normalized against **2-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C4'-H4'	-7.34	-21.59	-22.98	-30.85	-30.87	-18.03	-17.47	-21.65	-47.54	-13.58	-69.82	-28.20	-373.46	-2563.48	-18.53	114.02
C2-H2	-10.16	-1.42	-0.59	4.39	4.24	-3.60	-3.99	-1.37	14.49	-6.27	28.32	2.74	216.33	1570.37	-3.29	-85.09
C4'-P	-0.02	-0.11	-0.12	-0.16	-0.16	-0.09	-0.09	-0.11	-0.24	-0.07	-0.37	-0.15	-1.91	-12.91	-0.10	0.59
C1'-P	-0.75	-1.84	-1.97	-2.60	-2.57	-1.46	-1.46	-1.86	-3.86	-1.17	-6.21	-2.47	-31.68	-210.88	-1.67	9.88
C2-P	0.37	-0.19	-0.29	-0.09	-0.43	-0.10	-0.15	-0.24	-0.47	0.04	-0.52	-0.16	-0.16	-2.53	-0.17	0.12
C5-P	-0.34	-0.04	-0.04	0.02	-0.18	-0.12	-0.17	0.01	0.08	-0.06	0.55	0.00	1.84	3.36	-0.05	-0.41
C3-P	0.04	-0.13	-0.16	-0.14	-0.27	-0.09	-0.11	-0.14	-0.65	-0.02	-0.90	-0.15	-3.99	-28.42	-0.11	1.45
C4-P	-0.23	-0.19	-0.18	-0.22	-0.17	-0.15	-0.16	-0.05	-0.38	-0.07	-0.47	-0.06	-2.58	-18.03	-0.06	0.88
R		0.544	0.509	0.365	0.366	0.654	0.675	0.542	0.224	0.827	0.146	0.404	0.025	0.003	0.636	0.076
Q		0.435	0.424	0.476	0.416	0.447	0.422	0.421	0.531	0.484	0.533	0.437	0.621	0.634	0.395	0.628

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	Q	R	S	T	U
C4'-H4'	-7.34	-27.74	-13.34	-12.85	-14.70	230.27	-62.70
C2-H2	-10.16	2.33	-6.46	-6.73	-5.65	-156.63	24.03
C4'-P	-0.02	-0.14	-0.07	-0.07	-0.07	1.18	-0.32
C1'-P	-0.75	-2.25	-1.17	-1.13	-1.20	19.58	-5.28
C2-P	0.37	-0.06	-0.04	0.03	0.03	1.01	-0.33
C5-P	-0.34	-0.50	-0.08	-0.10	-0.33	-0.95	-0.27
C3-P	0.04	-0.18	-0.04	-0.02	-0.05	2.99	-0.32
C4-P	-0.23	-0.21	-0.03	-0.02	-0.10	1.63	-0.15
R		0.413	0.837	0.857	0.782	0.039	0.164
Q		0.428	0.449	0.476	0.414	0.639	0.475

Table S26: Theoretical (calculated) RDCs of conformers of **2-SR** derived from molecular docking after normal mode relaxation; normalized against **2-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C4'-H4'	-15.10	-18.60	-19.56	-20.68	-20.73	-17.38	-17.19	-20.32	-25.04	-16.07	-26.35	-19.93	-30.59	-31.22	-17.30	-33.38
C2-H2	-9.75	-3.97	-2.32	-0.31	-0.28	-6.08	-6.43	-0.98	7.38	-8.27	9.76	-1.58	17.15	18.22	-6.15	22.05
C4'-P	0.10	-0.10	-0.10	-0.11	-0.11	-0.09	-0.09	-0.11	-0.13	-0.08	-0.14	-0.11	-0.16	-0.16	-0.09	-0.18
C1'-P	-1.54	-1.62	-1.72	-1.78	-1.78	-1.46	-1.48	-1.76	-2.12	-1.39	-2.37	-1.77	-2.66	-2.63	-1.55	-2.94
C1-P	0.46	0.03	-0.05	-0.07	0.12	0.06	0.12	-0.11	0.23	0.06	0.17	0.01	0.16	0.19	0.05	0.21
C2-P	0.17	-0.09	-0.19	-0.03	-0.19	-0.04	-0.09	-0.24	-0.15	0.05	-0.09	-0.04	-0.04	-0.06	-0.09	0.03
C5-P	-0.17	-0.01	-0.01	0.03	-0.09	-0.10	-0.13	0.01	0.05	-0.07	0.20	-0.02	0.15	0.05	-0.03	0.15
C3-P	-0.01	-0.09	-0.11	-0.08	-0.15	-0.06	-0.08	-0.13	-0.30	-0.02	-0.28	-0.08	-0.33	-0.35	-0.08	-0.36
C4-P	-0.09	-0.14	-0.14	-0.14	-0.10	-0.13	-0.14	-0.05	-0.18	-0.09	-0.16	-0.04	-0.21	-0.22	-0.04	-0.22
R		0.920	0.877	0.823	0.822	0.964	0.97	0.84	0.626	0.993	0.577	0.858	0.456	0.443	0.966	0.399
Q		0.382	0.364	0.411	0.345	0.404	0.373	0.349	0.472	0.429	0.479	0.375	0.551	0.561	0.360	0.575

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	Q	R	S	T	U
C4'-H4'	-15.10	-20.03	-16.21	-15.00	-15.81	-34.44	-22.48
C2-H2	-9.75	-1.27	-8.13	-10.08	-8.66	23.76	2.85
C4'-P	0.10	-0.10	-0.09	-0.08	-0.08	-0.18	-0.12
C1'-P	-1.54	-1.68	-1.43	-1.32	-1.35	-3.02	-1.90
C1-P	0.46	0.47	0.07	0.10	0.34	0.02	-0.11
C2-P	0.17	0.02	-0.05	0.07	0.08	-0.16	-0.07
C5-P	-0.17	-0.28	-0.10	-0.09	-0.29	0.13	-0.08
C3-P	-0.01	-0.10	-0.06	-0.01	-0.04	-0.44	-0.10
C4-P	-0.09	-0.12	-0.04	-0.02	-0.08	-0.25	-0.05
R		0.851	0.992	0.999	0.996	0.38	0.736
Q		0.371	0.385	0.458	0.383	0.574	0.400

Table S27: Theoretical (calculated) RDCs of conformers of **2-SR** derived from molecular docking after normal mode relaxation; normalized against **2-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C4'-H4'	-7.34	-17.72	-20.06	-23.18	-23.37	-15.19	-14.85	-22.13	-45.83	-12.95	-59.58	-21.05	-257.63	-439.83	-15.12	346.89
C2-H2	-10.16	-3.79	-2.38	-0.34	-0.31	-5.31	-5.56	-1.07	13.51	-6.67	22.06	-1.66	144.40	256.60	-5.37	-229.17
C4'-P	-0.02	-0.09	-0.11	-0.12	-0.12	-0.08	-0.08	-0.12	-0.24	-0.07	-0.32	-0.11	-1.36	-2.28	-0.08	1.84
C1'-P	-0.75	-1.55	-1.77	-1.99	-2.00	-1.27	-1.28	-1.91	-3.88	-1.12	-5.36	-1.87	-22.40	-37.01	-1.35	30.56
C2-P	0.37	-0.09	-0.19	-0.03	-0.22	-0.04	-0.08	-0.26	-0.28	0.04	-0.20	-0.04	-0.36	-0.87	-0.07	-0.33
C5-P	-0.34	-0.01	-0.01	0.03	-0.10	-0.08	-0.11	0.01	0.09	-0.05	0.45	-0.02	1.23	0.63	-0.02	-1.53
C3-P	0.04	-0.08	-0.12	-0.09	-0.17	-0.05	-0.07	-0.14	-0.55	-0.02	-0.64	-0.09	-2.79	-4.90	-0.07	3.79
C4-P	-0.23	-0.13	-0.14	-0.15	-0.11	-0.11	-0.12	-0.06	-0.34	-0.07	-0.36	-0.04	-1.79	-3.08	-0.03	2.30
R		0.665	0.588	0.502	0.499	0.761	0.775	0.529	0.233	0.853	0.174	0.557	0.037	0.022	0.764	0.026
Q		0.449	0.429	0.482	0.410	0.469	0.435	0.419	0.539	0.499	0.548	0.450	0.620	0.630	0.428	0.644

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	Q	R	S	T	U
C4'-H4'	-7.34	-21.60	-13.13	-11.36	-12.62	200.46	-29.89
C2-H2	-10.16	-1.38	-6.59	-7.63	-6.91	-138.28	3.79
C4'-P	-0.02	-0.11	-0.07	-0.06	-0.07	1.06	-0.15
C1'-P	-0.75	-1.81	-1.16	-1.00	-1.07	17.56	-2.52
C2-P	0.37	0.02	-0.04	0.05	0.06	0.93	-0.09
C5-P	-0.34	-0.30	-0.08	-0.07	-0.23	-0.76	-0.10
C3-P	0.04	-0.11	-0.04	-0.01	-0.03	2.58	-0.14
C4-P	-0.23	-0.13	-0.03	-0.01	-0.07	1.44	-0.07
R		0.543	0.846	0.915	0.868	0.045	0.379
Q		0.435	0.452	0.531	0.446	0.642	0.474

Table S28: Theoretical (calculated) RDCs of conformers of **2-RR** derived from molecular docking; normalized against **2-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C4'-H4'	-15.10	-13.81	-13.33	-13.36	-13.43	-13.73	-14.60	-14.48	-13.36	-14.46	-18.23	-16.78	-13.35	-14.15	-14.14	-13.36
C2-H2	-9.75	-12.26	-13.04	-12.93	-12.88	-12.38	-10.95	-11.13	-13.00	-11.14	-4.09	-6.74	-12.90	-11.64	-11.70	-12.99
C4'-P	0.10	-0.07	-0.07	-0.07	-0.07	-0.07	-0.07	-0.07	-0.07	-0.07	-0.09	-0.09	-0.07	-0.07	-0.07	-0.07
C1'-P	-1.54	-1.06	-1.08	-1.10	-1.11	-1.11	-1.18	-1.20	-1.10	-1.20	-1.52	-1.41	-1.05	-1.16	-1.15	-1.12
C1-P	0.46	0.02	0.22	0.17	0.16	0.16	-0.09	0.01	0.27	0.05	0.24	0.15	0.15	0.08	0.08	0.20
C2-P	0.17	-0.25	-0.14	-0.11	-0.16	-0.21	-0.24	-0.21	-0.12	-0.21	0.23	0.17	-0.08	-0.20	-0.20	-0.11
C5-P	-0.17	0.15	0.07	0.11	0.09	0.07	0.18	0.13	0.04	0.11	0.21	0.21	0.13	0.10	0.09	0.09
C3-P	-0.01	-0.03	-0.04	-0.02	-0.03	-0.05	-0.05	-0.05	-0.04	-0.05	0.06	0.09	0.02	-0.05	-0.05	-0.03
C4-P	-0.09	0.01	-0.02	0.00	-0.01	-0.02	0.00	-0.01	-0.03	-0.02	0.04	0.06	0.05	-0.02	-0.02	-0.02
R		0.984	0.973	0.974	0.975	0.982	0.995	0.995	0.974	0.995	0.927	0.977	0.974	0.99	0.99	0.974
Q		0.488	0.449	0.467	0.455	0.426	0.429	0.386	0.438	0.370	0.414	0.480	0.577	0.390	0.393	0.451

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	Q	R	S	T	U
C4'-H4'	-15.10	-13.81	-15.70	-13.61	-13.50	-15.54	-17.26
C2-H2	-9.75	-12.40	-8.52	-12.43	-12.63	-9.15	-6.23
C4'-P	0.10	-0.07	-0.08	-0.07	-0.07	-0.08	-0.09
C1'-P	-1.54	-1.09	-1.32	-1.11	-1.08	-1.30	-1.39
C1-P	0.46	0.03	0.36	0.41	0.51	0.18	0.18
C2-P	0.17	-0.31	0.23	-0.04	-0.04	-0.17	-0.29
C5-P	-0.17	0.02	0.07	-0.03	-0.12	0.05	0.02
C3-P	-0.01	-0.08	0.09	-0.03	-0.03	-0.01	-0.04
C4-P	-0.09	-0.05	0.04	-0.04	-0.06	0.00	-0.02
R		0.983	0.996	0.981	0.979	0.998	0.967
Q		0.407	0.479	0.414	0.405	0.402	0.364

Table S29: Theoretical (calculated) RDCs of conformers of **2-RR** derived from molecular docking; normalized against **2-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C4'-H4'	-7.34	-9.75	-9.20	-9.25	-9.32	-9.67	-10.73	-10.59	-9.24	-10.59	-17.19	-14.21	-9.23	-10.20	-10.16	-9.22
C2-H2	-10.16	-8.65	-9.00	-8.96	-8.93	-8.72	-8.05	-8.14	-8.99	-8.15	-3.85	-5.71	-8.92	-8.39	-8.40	-8.97
C4'-P	-0.02	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.09	-0.07	-0.05	-0.05	-0.05	-0.05
C1'-P	-0.75	-0.75	-0.75	-0.76	-0.77	-0.79	-0.87	-0.88	-0.76	-0.88	-1.43	-1.19	-0.72	-0.83	-0.83	-0.77
C2-P	0.37	-0.17	-0.09	-0.08	-0.11	-0.15	-0.18	-0.15	-0.09	-0.15	0.21	0.15	-0.05	-0.14	-0.14	-0.08
C5-P	-0.34	0.11	0.05	0.08	0.06	0.05	0.13	0.10	0.03	0.08	0.20	0.18	0.09	0.07	0.07	0.06
C3-P	0.04	-0.02	-0.03	-0.02	-0.02	-0.03	-0.03	-0.03	-0.03	-0.04	0.06	0.08	0.01	-0.04	-0.03	-0.02
C4-P	-0.23	0.01	-0.01	0.00	-0.01	-0.02	0.00	-0.01	-0.02	-0.02	0.04	0.05	0.03	-0.02	-0.02	-0.01
R		0.965	0.978	0.977	0.976	0.968	0.936	0.941	0.978	0.941	0.678	0.795	0.977	0.953	0.954	0.978
Q		0.542	0.509	0.531	0.517	0.485	0.478	0.450	0.496	0.433	0.499	0.544	0.640	0.452	0.455	0.513

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	Q	R	S	T	U
C4'-H4'	-7.34	0.965	0.978	0.977	0.976	0.968	0.936
C2-H2	-10.16	0.542	0.509	0.531	0.517	0.485	0.478
C4'-P	-0.02	0.965	0.978	0.977	0.976	0.968	0.936
C1'-P	-0.75	0.542	0.509	0.531	0.517	0.485	0.478
C2-P	0.37	0.965	0.978	0.977	0.976	0.968	0.936
C5-P	-0.34	0.542	0.509	0.531	0.517	0.485	0.478
C3-P	0.04	0.965	0.978	0.977	0.976	0.968	0.936
C4-P	-0.23	0.542	0.509	0.531	0.517	0.485	0.478
R		0.967	0.867	0.970	0.973	0.884	0.767
Q		0.451	0.540	0.472	0.447	0.477	0.413

Table S30: Theoretical (calculated) RDCs of conformers of **2-RR** derived from molecular docking after normal mode relaxation; normalized against **2-SR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C4'-H4'	-15.10	-13.53	-13.32	-13.34	-13.45	-13.72	-15.01	-14.51	-13.32	-14.49	-18.24	-18.06	-13.31	-14.10	-14.09	-13.34
C2-H2	-9.75	-12.66	-13.07	-13.01	-12.85	-12.43	-10.11	-11.03	-13.02	-11.12	-4.11	-4.46	-12.93	-11.74	-11.76	-13.05
C4'-P	0.10	-0.07	-0.07	-0.07	-0.07	-0.07	-0.08	-0.07	-0.07	-0.07	-0.09	-0.09	-0.07	-0.07	-0.07	-0.07
C1'-P	-1.54	-1.10	-1.12	-1.11	-1.13	-1.16	-1.26	-1.22	-1.12	-1.21	-1.53	-1.52	-1.13	-1.17	-1.17	-1.14
C1-P	0.46	0.11	0.24	0.17	0.17	0.18	0.03	0.01	0.29	0.03	0.24	0.25	0.21	0.08	0.09	0.20
C2-P	0.17	-0.15	-0.14	-0.12	-0.17	-0.20	-0.13	-0.21	-0.13	-0.22	0.22	0.22	0.01	-0.20	-0.20	-0.13
C5-P	-0.17	0.13	0.06	0.12	0.08	0.06	0.18	0.14	0.03	0.11	0.21	0.20	0.12	0.10	0.09	0.09
C3-P	-0.01	-0.02	-0.04	-0.03	-0.04	-0.05	-0.03	-0.05	-0.04	-0.05	0.06	0.06	0.03	-0.05	-0.05	-0.04
C4-P	-0.09	0.01	-0.02	0.00	-0.02	-0.03	0.00	-0.01	-0.03	-0.02	0.03	0.03	0.04	-0.03	-0.03	-0.02
R		0.978	0.973	0.973	0.976	0.982	0.999	0.995	0.973	0.995	0.927	0.935	0.974	0.99	0.989	0.973
Q		0.481	0.439	0.461	0.443	0.417	0.388	0.375	0.426	0.371	0.409	0.413	0.566	0.384	0.384	0.444

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	Q	R	S	T	U
C4'-H4'	-15.10	-14.15	-16.75	-13.60	-14.05	-15.55	-15.65
C2-H2	-9.75	-11.71	-6.67	-12.45	-11.60	-9.13	-8.94
C4'-P	0.10	-0.07	-0.09	-0.07	-0.07	-0.08	-0.08
C1'-P	-1.54	-1.18	-1.43	-1.13	-1.18	-1.33	-1.32
C1-P	0.46	0.11	0.38	0.41	0.46	0.20	0.25
C2-P	0.17	-0.20	0.23	-0.04	0.02	-0.16	-0.16
C5-P	-0.17	0.05	0.10	-0.03	-0.03	0.04	0.00
C3-P	-0.01	-0.05	0.06	-0.03	-0.02	-0.01	-0.02
C4-P	-0.09	-0.04	0.03	-0.04	-0.04	0.00	-0.02
R		0.990	0.977	0.981	0.991	0.998	0.998
Q		0.375	0.412	0.409	0.400	0.400	0.389

Table S31: Theoretical (calculated) RDCs of conformers of **2-RR** derived from molecular docking after normal mode relaxation; normalized against **2-RR** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C4'-H4'	-7.34	-9.45	-9.19	-9.21	-9.34	-9.65	-11.34	-10.66	-9.21	-10.62	-17.16	-16.74	-9.21	-10.14	-10.12	-9.19
C2-H2	-10.16	-8.84	-9.02	-8.98	-8.93	-8.74	-7.64	-8.11	-9.00	-8.15	-3.87	-4.14	-8.94	-8.44	-8.44	-9.00
C4'-P	-0.02	-0.05	-0.05	-0.05	-0.05	-0.05	-0.06	-0.05	-0.05	-0.05	-0.09	-0.09	-0.05	-0.05	-0.05	-0.05
C1'-P	-0.75	-0.77	-0.77	-0.77	-0.79	-0.81	-0.95	-0.89	-0.78	-0.89	-1.44	-1.41	-0.78	-0.84	-0.84	-0.78
C2-P	0.37	-0.11	-0.10	-0.08	-0.12	-0.14	-0.10	-0.15	-0.09	-0.16	0.21	0.20	0.01	-0.15	-0.14	-0.09
C5-P	-0.34	0.09	0.04	0.08	0.06	0.04	0.14	0.10	0.02	0.08	0.20	0.18	0.08	0.07	0.07	0.06
C3-P	0.04	-0.01	-0.03	-0.02	-0.03	-0.04	-0.02	-0.04	-0.03	-0.04	0.05	0.06	0.02	-0.04	-0.04	-0.02
C4-P	-0.23	0.00	-0.01	0.00	-0.01	-0.02	0.00	-0.01	-0.02	-0.02	0.03	0.03	0.02	-0.02	-0.02	-0.01
R		0.973	0.979	0.978	0.975	0.968	0.914	0.939	0.978	0.941	0.679	0.695	0.978	0.955	0.956	0.978
Q		0.552	0.499	0.526	0.505	0.477	0.456	0.440	0.485	0.434	0.494	0.497	0.645	0.446	0.446	0.505

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs					
		Conformer					
		P	Q	R	S	T	U
C4'-H4'	-7.34	-10.17	-14.30	-9.57	-10.15	-12.19	-12.37
C2-H2	-10.16	-8.42	-5.70	-8.76	-8.38	-7.16	-7.06
C4'-P	-0.02	-0.05	-0.07	-0.05	-0.05	-0.06	-0.06
C1'-P	-0.75	-0.85	-1.22	-0.80	-0.85	-1.05	-1.04
C2-P	0.37	-0.15	0.20	-0.03	0.02	-0.13	-0.13
C5-P	-0.34	0.04	0.09	-0.02	-0.02	0.03	0.00
C3-P	0.04	-0.04	0.05	-0.02	-0.01	-0.01	-0.01
C4-P	-0.23	-0.03	0.02	-0.03	-0.03	0.00	-0.01
R		0.954	0.793	0.97	0.955	0.883	0.877
Q		0.436	0.494	0.468	0.461	0.476	0.460

Table S32: Theoretical (calculated) RDCs of conformers of **3-RS** derived from molecular docking; normalized against **3-A** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C3'-H3'	-8.64	-15.31	-15.42	-18.44	-16.82	-14.31	-14.54	-15.78	-14.08	-12.87	-4.71	-27.61	-23.65	-10.11	-6.81	-11.41
C6'-C6'	-10.03	-14.42	-14.73	-17.66	-16.12	-13.67	-13.79	-14.95	-13.39	-11.53	-4.12	-25.80	-22.28	-9.50	-6.08	-11.06
C4'-H4'	-13.93	-38.39	-41.67	-37.08	-31.80	-30.05	-30.44	-32.12	-30.79	-32.42	-39.74	-76.96	-59.62	-22.76	-52.58	-68.70
C5'-H5'	14.56	-14.76	-15.90	-14.19	-11.36	-9.76	-10.32	-12.36	-9.71	-10.83	2.10	-27.24	-22.97	4.60	1.23	3.91
C2-H2	-17.16	-27.52	-26.21	-24.93	-27.11	-28.87	-29.07	-29.03	-28.56	-29.94	-16.59	-1.77	-13.35	-21.74	-5.96	14.03
C6'-P	-0.16	-0.55	-0.58	-0.55	-0.50	-0.48	-0.48	-0.48	-0.49	-0.46	-0.21	-1.17	-0.88	-0.24	-0.28	-0.39
C4'-P	-0.21	-0.12	-0.13	-0.13	-0.11	-0.10	-0.10	-0.10	-0.10	-0.11	-0.12	-0.25	-0.19	-0.08	-0.15	-0.20
C5'-P	-0.02	-0.20	-0.21	-0.20	-0.17	-0.16	-0.16	-0.17	-0.17	-0.17	-0.12	-0.42	-0.31	-0.10	-0.16	-0.21
C3'P	-0.11	-0.12	-0.14	-0.14	-0.11	-0.10	-0.10	-0.11	-0.10	-0.11	-0.16	-0.26	-0.20	-0.09	-0.21	-0.28
C1-P	0.87	0.28	0.07	-0.28	0.03	0.51	0.56	0.19	0.16	0.59	-0.28	-1.14	-0.95	-0.22	-0.29	-0.55
C2-P	0.41	-0.81	-0.94	-0.77	-0.61	-0.39	-0.37	-0.56	-0.54	-0.41	-0.87	-2.14	-1.39	-0.31	-1.22	-1.82
C5-P	-0.07	-0.10	-0.08	0.15	0.11	-0.03	-0.06	0.07	-0.09	-0.07	0.12	-0.20	0.10	0.18	-0.02	0.16
C3-P	-0.07	-0.18	-0.21	-0.16	-0.13	-0.10	-0.09	-0.11	-0.07	-0.12	-0.11	-0.53	-0.32	0.09	-0.22	-0.41
C4-P	-0.14	-0.14	-0.14	-0.10	-0.09	-0.07	-0.08	-0.09	-0.11	-0.06	0.13	-0.31	-0.18	0.08	-0.13	-0.19
	R	0.630	0.605	0.642	0.695	0.716	0.708	0.681	0.714	0.668	0.702	0.359	0.456	0.914	0.562	0.407
	Q	0.423	0.409	0.406	0.441	0.458	0.455	0.448	0.456	0.447	0.389	0.365	0.367	0.471	0.372	0.392

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs							
		Conformer							
		P	Q	R	S	T	U	V	W
C3'-H3'	-8.64	-18.36	-54.82	-159.85	-78.45	658.63	-23.31	-21.45	-25.98
C6'-C6'	-10.03	-17.16	-52.33	-152.64	-73.07	614.60	-22.87	-21.15	-25.42
C4'-H4'	-13.93	-60.44	-199.58	-592.07	-294.86	2694.64	-49.83	-35.93	-98.02
C5'-H5'	14.56	3.48	-69.91	-224.32	-79.04	993.65	9.54	6.83	4.75
C2-H2	-17.16	13.04	66.63	281.60	149.63	-1541.04	16.99	1.49	50.76
C6'-P	-0.16	-0.74	-2.83	-8.33	-4.13	40.54	-0.33	-0.21	-0.67
C4'-P	-0.21	-0.19	-0.64	-1.96	-0.97	9.10	-0.16	-0.12	-0.30
C5'-P	-0.02	-0.28	-1.05	-3.14	-1.54	14.86	-0.17	-0.12	-0.33
C3'P	-0.11	-0.21	-0.64	-1.98	-0.99	9.04	-0.21	-0.16	-0.41
C1-P	0.87	-0.38	-4.54	-16.05	-7.28	74.08	-0.43	-0.28	-0.69
C2-P	0.41	-1.86	-5.99	-17.05	-8.73	79.40	-1.56	-1.15	-2.94
C5-P	-0.07	-0.13	-1.44	-3.17	-1.74	15.36	0.14	0.05	-0.81
C3-P	-0.07	-0.46	-1.69	-4.88	-2.45	22.56	-0.37	-0.28	-0.76
C4-P	-0.14	-0.27	-0.97	-2.43	-1.56	11.11	-0.17	-0.14	-0.56
R		0.446	0.130	0.041	0.082	0.008	0.472	0.650	0.248
Q		0.398	0.395	0.407	0.419	0.420	0.426	0.409	0.447

Table S33: Theoretical (calculated) RDCs of conformers of **3-RS** derived from molecular docking; normalized against **3-B** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C3'-H3'	-4.55	-8.40	-9.57	-9.56	-7.75	-6.56	-6.62	-7.12	-6.71	-6.35	-44.71	42.14	-40.74	-6.40	6.72	4.17
C6'-H6'	-4.44	-7.91	-9.14	-9.16	-7.42	-6.27	-6.28	-6.74	-6.38	-5.69	-39.05	39.38	-38.37	-6.02	6.00	4.04
C4'-H4'	1.86	-21.06	-25.87	-19.22	-14.64	-13.77	-13.86	-14.49	-14.68	-16.00	-377.03	117.46	-102.68	-14.40	51.86	25.12
C5'-H5'	-1.08	-8.10	-9.87	-7.36	-5.23	-4.47	-4.70	-5.58	-4.63	-5.35	19.92	41.58	-39.56	2.91	-1.21	-1.43
C2-H2	-7.25	-15.10	-16.27	-12.93	-12.49	-13.23	-13.24	-13.10	-13.61	-14.78	-157.37	2.70	-23.00	-13.76	5.88	-5.13
C6'-P	0.08	-0.30	-0.36	-0.29	-0.23	-0.22	-0.22	-0.22	-0.23	-0.23	-2.00	1.78	-1.52	-0.15	0.27	0.14
C4'-P	-0.07	-0.07	-0.08	-0.07	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-1.10	0.39	-0.33	-0.05	0.15	0.07
C5'-P	-0.04	-0.11	-0.13	-0.10	-0.08	-0.07	-0.07	-0.08	-0.08	-0.08	-1.15	0.63	-0.54	-0.06	0.16	0.08
C1'-P	0.00	-0.45	-0.54	-0.45	-0.35	-0.33	-0.33	-0.34	-0.34	-0.36	-5.91	2.58	-2.36	-0.30	0.80	0.42
C1-P	0.86	0.15	0.04	-0.15	0.01	0.24	0.25	0.08	0.07	0.29	-2.64	1.73	-1.63	-0.14	0.29	0.20
C2-P	0.21	-0.44	-0.58	-0.40	-0.28	-0.18	-0.17	-0.25	-0.26	-0.20	-8.30	3.27	-2.39	-0.19	1.20	0.67
C5-P	-0.29	-0.05	-0.05	0.08	0.05	-0.01	-0.03	0.03	-0.04	-0.04	1.18	0.30	0.18	0.12	0.02	-0.06
C4-P	-0.21	-0.07	-0.09	-0.05	-0.04	-0.03	-0.04	-0.04	-0.05	-0.03	1.25	0.48	-0.31	0.05	0.13	0.07
	R	0.376	0.318	0.406	0.495	0.511	0.509	0.495	0.490	0.456	0.024	0.077	0.087	0.469	0.184	0.359
	Q	0.468	0.453	0.453	0.491	0.509	0.506	0.497	0.508	0.497	0.452	0.398	0.404	0.550	0.423	0.436

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs							
		Conformer							
		P	Q	R	S	T	U	V	W
C3'-H3'	-4.55	10.04	6.54	5.09	4.76	3.90	18.40	-77.81	4.78
C6'-H6'	-4.44	9.38	6.24	4.86	4.43	3.64	18.06	-76.72	4.68
C4'-H4'	1.86	33.04	23.81	18.84	17.88	15.97	39.33	-130.36	18.04
C5'-H5'	-1.08	-1.90	8.34	7.14	4.79	5.89	-7.53	24.77	-0.87
C2-H2	-7.25	-7.13	-7.95	-8.96	-9.07	-9.13	-13.41	5.42	-9.34
C6'-P	0.08	0.40	0.34	0.27	0.25	0.24	0.26	-0.77	0.12
C4'-P	-0.07	0.11	0.08	0.06	0.06	0.05	0.12	-0.42	0.06
C5'-P	-0.04	0.15	0.12	0.10	0.09	0.09	0.13	-0.42	0.06
C1'-P	0.00	0.73	0.48	0.39	0.38	0.35	0.75	-2.37	0.36
C1-P	0.86	0.21	0.54	0.51	0.44	0.44	0.34	-1.01	0.13
C2-P	0.21	1.02	0.72	0.54	0.53	0.47	1.23	-4.18	0.54
C5-P	-0.29	0.07	0.17	0.10	0.11	0.09	-0.11	0.18	0.15
C4-P	-0.21	0.15	0.12	0.08	0.09	0.07	0.13	-0.52	0.10
	R	0.263	0.350	0.415	0.440	0.472	0.193	0.058	0.435
	Q	0.440	0.422	0.431	0.445	0.442	0.471	0.461	0.482

Table S34: Theoretical (calculated) RDCs of conformers of **3-RS** derived from molecular docking after normal mode relaxation; normalized against **3-A** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C3'-H3'	-8.64	-16.95	-16.81	-22.24	-20.69	-19.43	-19.64	-19.06	-19.24	-18.26	0.00	-24.14	-22.15	-11.45	0.04	-4.28
C6'-C6'	-10.03	-17.38	-17.49	-22.88	-21.13	-19.55	-19.77	-19.51	-19.52	-18.44	-1.29	-24.75	-22.73	-11.81	-1.63	-6.74
C4'-H4'	-13.93	-24.45	-26.36	-25.95	-23.29	-22.37	-22.36	-23.57	-22.58	-23.31	-37.68	-40.66	-32.23	-18.03	-50.74	-66.70
C5'-H5'	14.56	-4.51	-5.07	-3.58	-3.35	-2.76	-2.50	-3.37	-3.12	-2.47	2.01	-9.11	-6.17	6.73	1.08	3.42
C2-H2	-17.16	-24.04	-23.15	-16.82	-20.20	-21.45	-20.89	-21.37	-21.86	-21.31	-21.75	-10.52	-15.34	-21.13	-12.61	6.79
C6'-P	-0.16	-0.34	-0.36	-0.38	-0.36	-0.34	-0.34	-0.35	-0.37	-0.31	-0.26	-0.61	-0.45	-0.21	-0.33	-0.45
C4'-P	-0.21	-0.09	-0.10	-0.10	-0.09	-0.08	-0.08	-0.09	-0.09	-0.09	-0.12	-0.15	-0.12	-0.07	-0.16	-0.21
C5'-P	-0.02	-0.12	-0.13	-0.14	-0.13	-0.12	-0.12	-0.12	-0.13	-0.12	-0.13	-0.22	-0.17	-0.08	-0.18	-0.23
C3'P	-0.11	-0.11	-0.11	-0.13	-0.11	-0.10	-0.10	-0.11	-0.11	-0.11	-0.16	-0.17	-0.15	-0.09	-0.21	-0.28
C1-P	0.87	0.32	0.20	-0.07	0.16	0.54	0.57	0.28	0.24	0.60	-0.10	-0.51	-0.35	-0.03	-0.08	-0.34
C2-P	0.41	-0.35	-0.42	-0.30	-0.24	-0.08	-0.05	-0.19	-0.21	-0.07	-0.66	-1.03	-0.55	-0.11	-1.02	-1.66
C5-P	-0.07	0.06	0.06	0.26	0.23	0.11	0.10	0.19	0.08	0.08	0.23	0.05	0.15	0.23	0.07	0.27
C3-P	-0.07	-0.06	-0.07	-0.04	-0.03	-0.02	-0.01	-0.02	0.01	-0.03	-0.04	-0.22	-0.09	0.12	-0.16	-0.35
C4-P	-0.14	-0.05	-0.05	-0.02	-0.02	-0.01	-0.01	-0.02	-0.04	0.00	0.17	-0.11	-0.06	0.10	-0.09	-0.15
	R	0.801	0.788	0.757	0.791	0.811	0.812	0.803	0.809	0.819	0.695	0.608	0.704	0.956	0.571	0.433
	Q	0.438	0.412	0.380	0.419	0.447	0.445	0.425	0.427	0.428	0.387	0.349	0.367	0.465	0.364	0.374

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs							
		Conformer							
		P	Q	R	S	T	U	V	W
C3'-H3'	-8.64	-18.71	-32.75	-49.81	-38.66	-59.66	-16.72	-16.01	-15.30
C6'-C6'	-10.03	-19.93	-34.22	-52.26	-40.71	-63.09	-18.67	-17.50	-18.65
C4'-H4'	-13.93	-40.55	-87.46	-126.09	-110.50	-162.69	-49.29	-37.45	-81.10
C5'-H5'	14.56	4.91	-19.12	-31.30	-16.46	-40.44	8.83	5.34	6.89
C2-H2	-17.16	1.05	21.43	53.72	48.36	80.61	10.98	-3.08	32.41
C6'-P	-0.16	-0.47	-1.22	-1.69	-1.51	-2.34	-0.39	-0.28	-0.62
C4'-P	-0.21	-0.14	-0.31	-0.45	-0.39	-0.58	-0.16	-0.12	-0.26
C5'-P	-0.02	-0.18	-0.46	-0.65	-0.58	-0.88	-0.18	-0.14	-0.30
C3'P	-0.11	-0.17	-0.33	-0.50	-0.43	-0.64	-0.21	-0.17	-0.35
C1-P	0.87	-0.09	-2.20	-3.73	-2.96	-4.81	-0.26	-0.13	-0.41
C2-P	0.41	-1.24	-2.55	-3.35	-3.23	-4.44	-1.41	-1.06	-2.38
C5-P	-0.07	-0.02	-0.32	-0.32	-0.31	-0.45	0.23	0.13	-0.58
C3-P	-0.07	-0.30	-0.66	-0.88	-0.84	-1.17	-0.32	-0.25	-0.62
C4-P	-0.14	-0.17	-0.32	-0.35	-0.46	-0.45	-0.13	-0.12	-0.44
R		0.628	0.301	0.191	0.223	0.145	0.519	0.693	0.318
Q		0.368	0.370	0.396	0.398	0.405	0.387	0.358	0.421

Table S35: Theoretical (calculated) RDCs of conformers of **3-RS** derived from molecular docking after normal mode relaxation; normalized against **3-B** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C3'-H3'	-4.55	-7.39	-7.83	-10.45	-8.79	-8.17	-8.34	-8.29	-8.08	-8.15	0.00	-19.63	-12.60	-6.13	-0.05	1.66
C6'-H6'	-4.44	-7.58	-8.15	-10.74	-8.98	-8.22	-8.40	-8.48	-8.20	-8.23	-4.84	-20.13	-12.93	-6.32	1.81	2.61
C4'-H4'	1.86	-10.66	-12.29	-12.19	-9.90	-9.40	-9.50	-10.25	-9.49	-10.40	-141.28	-33.06	-18.33	-9.65	56.12	25.83
C5'-H5'	-1.08	-1.97	-2.36	-1.68	-1.42	-1.16	-1.06	-1.47	-1.31	-1.10	7.54	-7.40	-3.51	3.60	-1.19	-1.33
C2-H2	-7.25	-10.49	-10.79	-7.90	-8.58	-9.02	-8.87	-9.29	-9.18	-9.51	-81.57	-8.55	-8.72	-11.31	13.95	-2.63
C6'-P	0.08	-0.15	-0.17	-0.18	-0.15	-0.14	-0.14	-0.15	-0.15	-0.14	-0.98	-0.49	-0.26	-0.11	0.37	0.17
C4'-P	-0.07	-0.04	-0.04	-0.05	-0.04	-0.04	-0.04	-0.04	-0.04	-0.04	-0.46	-0.12	-0.07	-0.04	0.17	0.08
C5'-P	-0.04	-0.05	-0.06	-0.07	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.51	-0.18	-0.09	-0.04	0.19	0.09
C1'-P	0.00	-0.29	-0.33	-0.38	-0.31	-0.29	-0.29	-0.31	-0.30	-0.30	-2.85	-0.90	-0.53	-0.27	1.02	0.49
C1-P	0.86	0.14	0.09	-0.03	0.07	0.23	0.24	0.12	0.10	0.27	-0.37	-0.41	-0.20	-0.02	0.09	0.13
C2-P	0.21	-0.15	-0.20	-0.14	-0.10	-0.04	-0.02	-0.08	-0.09	-0.03	-2.48	-0.84	-0.31	-0.06	1.13	0.64
C5-P	-0.29	0.03	0.03	0.12	0.10	0.05	0.04	0.08	0.03	0.04	0.87	0.04	0.09	0.12	-0.07	-0.10
C4-P	-0.21	-0.02	-0.03	-0.01	-0.01	0.00	-0.01	-0.01	-0.02	0.00	0.65	-0.09	-0.03	0.05	0.10	0.06
	R	0.601	0.555	0.528	0.609	0.631	0.625	0.606	0.630	0.601	0.059	0.244	0.405	0.580	0.167	0.361
	Q	0.516	0.489	0.456	0.496	0.524	0.522	0.502	0.507	0.506	0.490	0.412	0.436	0.594	0.444	0.441

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs							
		Conformer							
		P	Q	R	S	T	U	V	W
C3'-H3'	-4.55	530.15	14.49	10.46	8.29	8.11	13.51	-84.13	3.71
C6'-H6'	-4.44	564.80	15.14	10.98	8.72	8.57	15.08	-91.97	4.52
C4'-H4'	1.86	1148.80	38.70	26.48	23.68	22.11	39.83	-196.82	19.65
C5'-H5'	-1.08	-139.00	8.46	6.57	3.53	5.50	-7.14	28.05	-1.67
C2-H2	-7.25	-29.68	-9.48	-11.28	-10.36	-10.95	-8.88	-16.19	-7.85
C6'-P	0.08	13.44	0.54	0.35	0.32	0.32	0.32	-1.48	0.15
C4'-P	-0.07	3.90	0.14	0.09	0.08	0.08	0.13	-0.65	0.06
C5'-P	-0.04	5.17	0.20	0.14	0.12	0.12	0.15	-0.73	0.07
C1'-P	0.00	28.88	0.92	0.64	0.57	0.55	0.83	-3.95	0.42
C1-P	0.86	2.63	0.98	0.78	0.63	0.65	0.21	-0.68	0.10
C2-P	0.21	34.99	1.13	0.70	0.69	0.60	1.14	-5.55	0.58
C5-P	-0.29	0.43	0.14	0.07	0.07	0.06	-0.18	0.68	0.14
C4-P	-0.21	4.85	0.14	0.07	0.10	0.06	0.11	-0.61	0.11
	R	0.007	0.219	0.294	0.335	0.346	0.207	0.043	0.423
	Q	0.440	0.416	0.433	0.441	0.439	0.460	0.443	0.476

Table S36: Theoretical (calculated) RDCs of conformers of **3-RR** derived from molecular docking; normalized against **3-A** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C3'-H3'	-8.64	-20.43	-22.66	-25.42	-39.20	-27.95	-25.16	-21.21	-63.55	-23.52	-18.79	-21.08	-47.25	-5.29	-103.15	-109.18
C6'-C6'	-10.03	-20.26	-22.02	-23.58	-37.01	-26.64	-23.95	-20.65	-62.48	-22.20	-18.02	-19.56	-45.91	-5.31	-99.75	-106.29
C4'-H4'	-13.93	-84.22	-60.69	-64.80	-96.20	-53.60	-47.63	-47.40	-45.13	-41.65	-62.52	-101.19	-122.29	-126.16	-106.48	-109.24
C5'-H5'	14.56	0.11	-0.59	-0.57	5.85	4.52	4.20	4.41	-1.43	6.14	0.41	-7.27	5.02	-11.49	4.65	3.85
C2-H2	-17.16	30.87	12.98	17.36	62.38	17.09	10.38	7.07	38.00	6.57	11.76	34.16	90.03	34.56	128.29	135.37
C6'-P	-0.16	-0.95	-0.73	-0.80	-1.19	-0.69	-0.59	-0.56	-0.61	-0.67	-0.65	-1.03	-1.00	-1.65	-1.65	-1.69
C4'-P	-0.21	-0.28	-0.21	-0.22	-0.32	-0.20	-0.17	-0.17	-0.18	-0.16	-0.21	-0.34	-0.45	-0.49	-0.42	-0.43
C5'-P	-0.02	-0.38	-0.29	-0.31	-0.45	-0.27	-0.23	-0.22	-0.22	-0.22	-0.27	-0.44	-0.49	-0.67	-0.55	-0.57
C3'P	-0.11	-0.34	-0.25	-0.25	-0.37	-0.25	-0.22	-0.21	-0.26	-0.18	-0.26	-0.43	-0.63	-0.57	-0.52	-0.54
C1-P	0.87	0.30	0.02	-0.28	-0.21	0.02	0.01	0.15	-0.67	0.52	0.25	0.22	0.11	-2.00	-1.06	-0.91
C2-P	0.41	-1.20	-1.06	-0.93	-0.57	-1.05	-0.99	-0.93	0.33	-0.70	-1.03	-1.50	-1.70	-2.74	-0.20	-0.10
C5-P	-0.07	-1.28	-0.84	-1.26	-1.86	-0.69	-0.54	-0.55	-0.66	-0.39	-0.73	-1.62	-2.70	0.54	1.08	0.97
C3-P	-0.07	-0.99	-0.55	-0.47	-0.63	-0.80	-0.76	-0.72	-0.20	-0.64	-0.87	-1.24	-1.33	-1.68	-1.58	-1.65
C4-P	-0.14	-0.85	-0.72	-0.66	-1.03	-0.82	-0.61	-0.57	-0.49	-0.56	-0.74	-1.47	-1.25	-0.21	-0.58	-0.87
	R	0.306	0.434	0.403	0.228	0.446	0.507	0.540	0.280	0.570	0.438	0.266	0.171	0.220	0.131	0.125
	Q	0.404	0.391	0.403	0.473	0.403	0.399	0.387	0.495	0.407	0.382	0.392	0.461	0.347	0.545	0.555

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs													
		Conformer													
		P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
C3'-H3'	-8.64	-104.34	-130.03	90.65	-19.84	-23.83	-15.43	-18.34	-40.40	-68.55	-18.04	-113.52	-15.22	-23.46	-91.09
C6'-C6'	-10.03	-101.87	-125.29	51.54	-18.62	-22.76	-13.69	-17.08	-39.63	-68.41	-17.41	-109.27	-14.26	-21.99	-90.71
C4'-H4'	-13.93	-281.50	-135.84	3470.80	-42.43	-34.99	-84.49	-27.31	-34.13	-54.00	-38.15	-106.84	-30.82	-53.86	-71.78
C5'-H5'	14.56	-4.59	4.82	747.30	4.13	5.30	-0.55	6.16	-0.75	-3.29	-6.58	-9.53	1.76	6.86	5.74
C2-H2	-17.16	250.28	173.36	-1905.39	1.32	0.84	23.31	-9.23	9.07	47.95	-15.47	120.57	-14.18	16.83	92.61
C6'-P	-0.16	-3.48	-2.19	32.57	-0.47	-0.39	-0.97	-0.38	-0.44	-0.64	-0.55	-1.19	-0.46	-0.59	-1.07
C4'-P	-0.21	-0.92	-0.54	11.80	-0.15	-0.13	-0.30	-0.10	-0.14	-0.21	-0.14	-0.41	-0.11	-0.18	-0.30
C5'-P	-0.02	-1.31	-0.72	14.56	-0.19	-0.16	-0.39	-0.13	-0.16	-0.25	-0.20	-0.48	-0.16	-0.24	-0.37
C3'P	-0.11	-1.03	-0.68	15.31	-0.17	-0.17	-0.37	-0.12	-0.19	-0.31	-0.16	-0.58	-0.12	-0.22	-0.41
C1-P	0.87	-1.19	-0.89	24.08	0.01	0.27	-0.56	-0.29	-0.08	-0.66	-0.12	-2.00	0.55	0.07	-0.88
C2-P	0.41	-3.42	0.62	63.51	-0.53	-0.74	-2.07	-0.19	0.30	-0.10	-0.33	-1.00	0.16	-0.16	-0.60
C5-P	-0.07	-4.39	1.72	22.44	-0.93	-0.29	-0.85	-0.07	-0.49	-0.61	-0.12	-0.58	-0.25	-1.28	0.45
C3-P	-0.07	-2.64	-1.79	53.92	-0.27	-0.62	-1.44	-0.11	-0.09	-0.35	-0.16	-0.84	-0.08	-0.27	-1.37
C4-P	-0.14	-2.05	-0.79	38.01	-0.31	-0.51	-0.94	-0.05	-0.17	-0.29	-0.12	-0.47	-0.11	-0.42	-0.53
R		0.074	0.105	0.006	0.612	0.644	0.328	0.821	0.466	0.246	0.684	0.130	0.811	0.454	0.167
Q		0.524	0.546	0.441	0.366	0.373	0.365	0.360	0.428	0.496	0.337	0.521	0.366	0.395	0.536

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs				
		Conformer				
		AD	AE	AF	AG	AH
C3'-H3'	-8.64	-12.36	-20.15	-11.01	-25.21	-120.43
C6'-C6'	-10.03	-11.57	-18.51	-9.24	-23.34	-113.33
C4'-H4'	-13.93	-48.47	-55.63	-80.18	-59.62	-109.53
C5'-H5'	14.56	4.26	4.80	-3.17	7.15	-6.87
C2-H2	-17.16	-0.38	12.62	13.73	22.68	130.84
C6'-P	-0.16	-0.46	-0.55	-0.72	-0.81	-1.24
C4'-P	-0.21	-0.16	-0.19	-0.27	-0.22	-0.43
C5'-P	-0.02	-0.20	-0.24	-0.33	-0.30	-0.50
C3'P	-0.11	-0.19	-0.23	-0.35	-0.26	-0.61
C1-P	0.87	0.10	0.12	1.02	-0.22	-1.83
C2-P	0.41	-0.12	-0.12	-0.81	-1.35	-1.39
C5-P	-0.07	-0.32	-1.32	-0.94	-0.64	-0.47
C3-P	-0.07	-0.20	-0.26	-0.91	-1.09	-1.15
C4-P	-0.14	-0.16	-0.43	-0.79	-0.72	-0.52
	R	0.587	0.470	0.357	0.405	0.123
	Q	0.350	0.377	0.360	0.389	0.522

Table S37: Theoretical (calculated) RDCs of conformers of **3-RR** derived from molecular docking; normalized against **3-B** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**	**K**	**L**	**M**	**N**	**O**
C3'-H3'	-4.55	5.32	15.59	14.42	7.54	25.79	43.62	34.64	-105.03	124.70	10.79	4.44	6.24	0.75	19.40	20.09
C6'-H6'	-4.44	5.28	15.16	13.38	7.12	24.58	41.51	33.74	-103.26	117.69	10.34	4.12	6.06	0.76	18.76	19.56
C4'-H4'	1.86	21.93	41.78	36.76	18.51	49.46	82.57	77.43	-74.60	220.83	35.89	21.30	16.15	18.00	20.02	20.10
C5'-H5'	-1.08	-0.03	0.41	0.32	-1.13	-4.17	-7.28	-7.20	-2.36	-32.56	-0.23	1.53	-0.66	1.64	-0.87	-0.71
C2-H2	-7.25	-8.04	-8.93	-9.85	-12.00	-15.77	-17.99	-11.55	62.81	-34.85	-6.75	-7.19	-11.89	-4.93	-24.12	-24.91
C6'-P	0.08	0.25	0.50	0.45	0.23	0.63	1.02	0.92	-1.00	3.54	0.38	0.22	0.13	0.23	0.31	0.31
C4'-P	-0.07	0.07	0.14	0.13	0.06	0.19	0.30	0.28	-0.30	0.82	0.12	0.07	0.06	0.07	0.08	0.08
C5'-P	-0.04	0.10	0.20	0.18	0.09	0.24	0.40	0.36	-0.36	1.19	0.15	0.09	0.07	0.10	0.10	0.10
C1'-P	0.00	0.54	1.03	0.85	0.44	1.40	2.28	2.08	-2.59	6.54	0.91	0.54	0.38	0.52	0.67	0.68
C1-P	0.86	-0.08	-0.02	0.16	0.04	-0.02	-0.03	-0.24	-1.10	-2.77	-0.14	-0.05	-0.01	0.29	0.20	0.17
C2-P	0.21	0.31	0.73	0.53	0.11	0.97	1.72	1.52	0.54	3.72	0.59	0.32	0.23	0.39	0.04	0.02
C5-P	-0.29	0.33	0.58	0.72	0.36	0.63	0.94	0.89	-1.08	2.09	0.42	0.34	0.36	-0.08	-0.20	-0.18
C4-P	-0.21	0.22	0.49	0.38	0.20	0.76	1.06	0.93	-0.80	2.99	0.42	0.31	0.16	0.03	0.11	0.16
	R	0.385	0.204	0.227	0.381	0.154	0.094	0.107	0.055	0.035	0.246	0.406	0.422	0.498	0.224	0.218
	Q	0.440	0.429	0.441	0.508	0.442	0.440	0.430	0.529	0.453	0.421	0.425	0.492	0.381	0.576	0.586

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs													
		Conformer													
		P	**Q**	**R**	**S**	**T**	**U**	**V**	**W**	**X**	**Y**	**Z**	**AA**	**AB**	**AC**
C3'-H3'	-4.55	4.97	17.04	0.34	156.23	-45.13	4.06	-16.47	-30.66	2627.63	-15.53	28.49	-13.47	16.42	41.20
C6'-H6'	-4.44	4.85	16.42	0.19	146.61	-43.10	3.61	-15.33	-30.08	2622.23	-14.99	27.43	-12.61	15.39	41.03
C4'-H4'	1.86	13.40	17.80	12.84	334.13	-66.26	22.24	-24.52	-25.91	2069.83	-32.85	26.82	-27.26	37.70	32.46
C5'-H5'	-1.08	0.22	-0.63	2.76	-32.52	10.04	0.14	5.53	-0.57	125.98	-5.66	2.39	1.55	-4.80	-2.60
C2-H2	-7.25	-11.91	-22.72	-7.05	-10.38	1.59	-6.14	-8.28	6.89	-1837.95	-13.31	-30.26	-12.54	-11.78	-41.88
C6'-P	0.08	0.17	0.29	0.12	3.70	-0.74	0.25	-0.34	-0.33	24.64	-0.48	0.30	-0.40	0.41	0.48
C4'-P	-0.07	0.04	0.07	0.04	1.14	-0.25	0.08	-0.09	-0.10	8.21	-0.12	0.10	-0.10	0.13	0.14
C5'-P	-0.04	0.06	0.09	0.05	1.50	-0.30	0.10	-0.12	-0.12	9.46	-0.17	0.12	-0.14	0.17	0.17
C1'-P	0.00	0.31	0.62	0.34	7.95	-1.93	0.61	-0.73	-0.85	68.72	-0.91	0.84	-0.72	0.90	1.24
C1-P	0.86	0.06	0.12	0.09	-0.08	0.52	0.15	-0.26	-0.06	25.43	-0.11	0.50	0.49	-0.05	0.40
C2-P	0.21	0.16	-0.08	0.23	4.18	-1.41	0.55	-0.17	0.23	3.94	-0.28	0.25	0.15	0.11	0.27
C5-P	-0.29	0.21	-0.23	0.08	7.33	-0.55	0.22	-0.06	-0.37	23.37	-0.11	0.14	-0.22	0.90	-0.20
C4-P	-0.21	0.10	0.10	0.14	2.41	-0.97	0.25	-0.04	-0.13	11.22	-0.11	0.12	-0.10	0.30	0.24
R		0.477	0.247	0.616	0.025	0.110	0.399	0.297	0.200	0.002	0.260	0.166	0.298	0.210	0.119
Q		0.554	0.576	0.469	0.435	0.443	0.419	0.449	0.483	0.536	0.406	0.555	0.449	0.457	0.601

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs				
		Conformer				
		AD	AE	AF	AG	AH
C3'-H3'	-4.55	15.31	13.83	3.43	12.68	27.37
C6'-H6'	-4.44	14.32	12.71	2.88	11.75	25.76
C4'-H4'	1.86	60.01	38.18	24.95	30.00	24.89
C5'-H5'	-1.08	-5.27	-3.29	0.99	-3.60	1.56
C2-H2	-7.25	0.46	-8.66	-4.27	-11.41	-29.74
C6'-P	0.08	0.57	0.38	0.22	0.41	0.28
C4'-P	-0.07	0.20	0.13	0.08	0.11	0.10
C5'-P	-0.04	0.25	0.16	0.10	0.15	0.11
C1'-P	0.00	1.26	0.87	0.61	0.87	0.81
C1-P	0.86	-0.12	-0.09	-0.32	0.11	0.42
C2-P	0.21	0.15	0.09	0.25	0.68	0.32
C5-P	-0.29	0.40	0.91	0.29	0.32	0.11
C4-P	-0.21	0.19	0.30	0.25	0.36	0.12
R		0.153	0.221	0.370	0.260	0.173
Q		0.426	0.441	0.411	0.448	0.555

Table S38: Theoretical (calculated) RDCs of conformers of **3-RR** derived from molecular docking after normal mode relaxation; normalized against **3-A** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
C3'-H3'	-8.64	-18.96	-21.19	-20.98	-29.36	-26.08	-24.68	-21.54	-41.86	-28.51	-17.95	-16.05	-29.91	-15.03	-71.19	-77.12
C6'-C6'	-10.03	-21.62	-22.91	-22.19	-30.47	-27.72	-26.07	-23.14	-42.51	-29.18	-19.77	-18.58	-32.90	-18.43	-70.95	-77.04
C4'-H4'	-13.93	-65.25	-46.94	-44.16	-65.64	-44.75	-40.90	-40.89	-35.43	-36.09	-52.10	-75.79	-106.97	-75.47	-67.87	-72.56
C5'-H5'	14.56	8.02	2.39	4.57	8.40	8.93	7.94	7.75	2.56	5.20	6.11	5.28	12.52	0.92	12.44	11.83
C2-H2	-17.16	24.62	5.76	5.49	34.31	15.89	10.42	7.49	16.05	7.03	11.13	27.00	72.50	21.11	79.55	88.09
C6'-P	-0.16	-0.70	-0.53	-0.52	-0.81	-0.54	-0.48	-0.46	-0.51	-0.57	-0.51	-0.72	-0.92	-0.87	-1.06	-1.13
C4'-P	-0.21	-0.23	-0.17	-0.16	-0.23	-0.17	-0.16	-0.15	-0.15	-0.14	-0.18	-0.26	-0.40	-0.30	-0.28	-0.30
C5'-P	-0.02	-0.29	-0.21	-0.21	-0.31	-0.22	-0.19	-0.19	-0.18	-0.20	-0.22	-0.32	-0.44	-0.37	-0.36	-0.38
C3'P	-0.11	-0.29	-0.21	-0.19	-0.27	-0.22	-0.20	-0.20	-0.20	-0.18	-0.24	-0.35	-0.55	-0.39	-0.37	-0.39
C1-P	0.87	0.54	0.22	0.02	0.00	0.24	0.23	0.35	-0.29	0.62	0.46	0.52	0.54	-1.11	-0.27	-0.17
C2-P	0.41	-0.70	-0.70	-0.50	-0.20	-0.75	-0.74	-0.69	0.47	-0.54	-0.69	-0.86	-1.21	-1.29	0.23	0.32
C5-P	-0.07	-1.00	-0.67	-0.93	-1.21	-0.60	-0.48	-0.49	-0.31	-0.24	-0.62	-1.28	-2.37	0.68	0.93	0.88
C3-P	-0.07	-0.74	-0.41	-0.30	-0.41	-0.67	-0.67	-0.63	-0.06	-0.58	-0.71	-0.87	-1.11	-0.81	-0.91	-0.98
C4-P	-0.14	-0.68	-0.59	-0.48	-0.73	-0.74	-0.56	-0.52	-0.28	-0.51	-0.63	-1.15	-1.09	0.12	-0.27	-0.47
	R	0.386	0.541	0.566	0.341	0.486	0.540	0.573	0.427	0.557	0.498	0.345	0.208	0.359	0.198	0.182
	Q	0.396	0.372	0.373	0.440	0.399	0.392	0.378	0.451	0.408	0.371	0.387	0.450	0.338	0.557	0.566

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs													
		Conformer													
		P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
C3'-H3'	-8.64	-46.66	-76.33	52.63	-18.37	-23.36	-14.68	-16.85	-38.08	-69.84	-17.66	-115.04	-14.98	-20.67	-92.23
C6'-C6'	-10.03	-49.06	-75.56	170.02	-19.57	-24.57	-16.70	-17.21	-38.90	-70.60	-18.63	-114.47	-15.24	-21.81	-93.53
C4'-H4'	-13.93	-120.94	-76.54	5183.48	-41.07	-35.36	-86.57	-27.55	-33.46	-55.84	-37.97	-108.65	-31.78	-51.15	-73.18
C5'-H5'	14.56	12.36	12.25	1034.75	4.09	5.54	-0.34	6.24	-0.92	-4.77	-7.25	-11.07	1.54	6.95	5.40
C2-H2	-17.16	98.21	90.73	-2941.39	0.14	2.07	26.44	-9.39	7.07	49.16	-16.06	124.17	-13.20	13.57	95.67
C6'-P	-0.16	-1.50	-1.21	48.46	-0.45	-0.39	-1.00	-0.38	-0.43	-0.66	-0.55	-1.20	-0.46	-0.55	-1.08
C4'-P	-0.21	-0.42	-0.32	17.81	-0.14	-0.13	-0.31	-0.10	-0.13	-0.22	-0.14	-0.42	-0.11	-0.18	-0.31
C5'-P	-0.02	-0.57	-0.41	21.86	-0.19	-0.16	-0.41	-0.13	-0.16	-0.26	-0.20	-0.49	-0.16	-0.23	-0.38
C3'P	-0.11	-0.49	-0.41	23.11	-0.17	-0.18	-0.38	-0.12	-0.19	-0.32	-0.16	-0.59	-0.12	-0.21	-0.43
C1-P	0.87	-0.31	0.00	32.56	0.02	0.28	-0.54	-0.29	-0.05	-0.67	-0.08	-2.10	0.59	0.07	-0.90
C2-P	0.41	-1.26	0.80	94.56	-0.49	-0.75	-2.12	-0.19	0.33	-0.06	-0.32	-1.01	0.20	-0.13	-0.68
C5-P	-0.07	-1.64	1.16	32.71	-0.91	-0.27	-0.88	-0.07	-0.48	-0.64	-0.15	-0.59	-0.26	-1.23	0.45
C3-P	-0.07	-1.14	-0.80	80.26	-0.26	-0.63	-1.47	-0.11	-0.08	-0.36	-0.16	-0.88	-0.08	-0.26	-1.42
C4-P	-0.14	-0.85	-0.28	56.74	-0.30	-0.51	-0.96	-0.05	-0.17	-0.31	-0.13	-0.49	-0.11	-0.41	-0.55
R		0.168	0.179	0.005	0.631	0.630	0.316	0.827	0.486	0.240	0.682	0.125	0.795	0.486	0.162
Q		0.507	0.557	0.448	0.368	0.383	0.370	0.360	0.424	0.498	0.336	0.528	0.361	0.390	0.568

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs				
		Conformer				
		AD	AE	AF	AG	AH
C3'-H3'	-8.64	-12.67	-17.52	-9.26	-24.61	-118.74
C6'-C6'	-10.03	-14.32	-18.90	-11.66	-25.42	-115.43
C4'-H4'	-13.93	-50.03	-54.49	-80.12	-60.89	-110.48
C5'-H5'	14.56	4.11	4.70	-2.88	7.44	-7.66
C2-H2	-17.16	2.46	10.73	14.55	24.60	131.06
C6'-P	-0.16	-0.46	-0.53	-0.72	-0.82	-1.25
C4'-P	-0.21	-0.16	-0.19	-0.27	-0.22	-0.44
C5'-P	-0.02	-0.21	-0.23	-0.33	-0.31	-0.50
C3'P	-0.11	-0.19	-0.22	-0.36	-0.27	-0.62
C1-P	0.87	0.10	0.15	1.05	-0.20	-1.83
C2-P	0.41	-0.08	-0.08	-0.81	-1.39	-1.34
C5-P	-0.07	-0.34	-1.31	-0.95	-0.65	-0.45
C3-P	-0.07	-0.21	-0.25	-0.91	-1.10	-1.17
C4-P	-0.14	-0.17	-0.43	-0.79	-0.73	-0.52
R		0.559	0.487	0.356	0.394	0.122
Q		0.356	0.375	0.365	0.398	0.522

Table S39: Theoretical (calculated) RDCs of conformers of **3-RR** derived from molecular docking after normal mode relaxation; normalized against **3-B** experimental values.

Atoms	Experimental RDCs	Theoretical Normalized RDCs														
		Conformer														
		A	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**	**K**	**L**	**M**	**N**	**O**
C3'-H3'	-4.55	7.18	52.98	66.26	11.30	38.32	99.57	79.21	-45.39	-58.91	14.38	4.62	4.33	4.87	26.66	25.79
C6'-H6'	-4.44	8.19	57.28	70.07	11.73	40.72	105.16	85.09	-46.09	-60.28	15.84	5.35	4.76	5.97	26.58	25.76
C4'-H4'	1.86	24.73	117.35	139.44	25.26	65.73	165.00	150.34	-38.42	-74.57	41.72	21.83	15.49	24.44	25.42	24.27
C5'-H5'	-1.08	-3.04	-5.97	-14.44	-3.23	-13.11	-32.05	-28.50	2.78	10.74	-4.90	-1.52	-1.81	-0.30	-4.66	-3.96
C2-H2	-7.25	-9.33	-14.39	-17.32	-13.20	-23.34	-42.05	-27.53	17.41	14.52	-8.91	-7.78	-10.50	-6.84	-29.79	-29.46
C6'-P	0.08	0.27	1.33	1.64	0.31	0.80	1.94	1.68	-0.56	-1.18	0.41	0.21	0.13	0.28	0.40	0.38
C4'-P	-0.07	0.09	0.42	0.51	0.09	0.26	0.63	0.56	-0.16	-0.30	0.14	0.08	0.06	0.10	0.11	0.10
C5'-P	-0.04	0.11	0.54	0.66	0.12	0.32	0.77	0.68	-0.20	-0.40	0.17	0.09	0.06	0.12	0.13	0.13
C1'-P	0.00	0.65	3.04	3.55	0.65	1.98	4.89	4.30	-1.37	-2.48	1.10	0.56	0.38	0.72	0.93	0.89
C1-P	0.86	-0.21	-0.55	-0.07	0.00	-0.36	-0.92	-1.29	-0.31	1.28	-0.37	-0.15	-0.08	0.36	0.10	0.06
C2-P	0.21	0.27	1.75	1.59	0.08	1.10	3.00	2.53	0.51	-1.12	0.55	0.25	0.18	0.42	-0.09	-0.11
C5-P	-0.29	0.38	1.67	2.95	0.47	0.88	1.94	1.81	-0.33	-0.50	0.50	0.37	0.34	-0.22	-0.35	-0.29
C4-P	-0.21	0.26	1.48	1.53	0.28	1.09	2.27	1.91	-0.31	-1.06	0.51	0.33	0.16	-0.04	0.10	0.16
	R	0.328	0.071	0.058	0.285	0.106	0.043	0.050	0.128	0.087	0.201	0.387	0.462	0.358	0.170	0.175
	Q	0.452	0.435	0.439	0.494	0.461	0.457	0.446	0.506	0.471	0.435	0.442	0.495	0.397	0.600	0.607

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs													
		Conformer													
		P	**Q**	**R**	**S**	**T**	**U**	**V**	**W**	**X**	**Y**	**Z**	**AA**	**AB**	**AC**
C3'-H3'	-4.55	5.82	22.30	0.13	1567.86	-49.14	3.65	-15.91	-27.86	1536.37	-14.15	28.41	-14.23	17.20	39.53
C6'-H6'	-4.44	6.12	22.08	0.41	1670.18	-51.69	4.16	-16.24	-28.47	1553.28	-14.93	28.27	-14.48	18.14	40.09
C4'-H4'	1.86	15.08	22.36	12.63	3504.94	-74.40	21.55	-26.00	-24.49	1228.55	-30.43	26.83	-30.19	42.56	31.36
C5'-H5'	-1.08	-1.54	-3.58	2.52	-349.30	11.66	0.08	5.89	-0.67	105.05	-5.81	2.73	1.46	-5.78	-2.32
C2-H2	-7.25	-12.24	-26.51	-7.17	-11.79	4.36	-6.58	-8.86	5.17	-1081.56	-12.87	-30.66	-12.55	-11.29	-41.00
C6'-P	0.08	0.19	0.35	0.12	38.57	-0.82	0.25	-0.35	-0.31	14.49	-0.44	0.30	-0.44	0.46	0.46
C4'-P	-0.07	0.05	0.09	0.04	12.11	-0.28	0.08	-0.09	-0.10	4.88	-0.11	0.10	-0.11	0.15	0.13
C5'-P	-0.04	0.07	0.12	0.05	15.79	-0.33	0.10	-0.13	-0.12	5.66	-0.16	0.12	-0.16	0.19	0.16
C1'-P	0.00	0.38	0.81	0.33	82.97	-2.18	0.59	-0.75	-0.80	40.22	-0.85	0.83	-0.78	1.00	1.20
C1-P	0.86	0.04	0.00	0.08	-1.39	0.59	0.13	-0.28	-0.04	14.77	-0.07	0.52	0.56	-0.06	0.39
C2-P	0.21	0.16	-0.23	0.23	41.90	-1.58	0.53	-0.18	0.24	1.34	-0.26	0.25	0.19	0.11	0.29
C5-P	-0.29	0.20	-0.34	0.08	77.65	-0.57	0.22	-0.07	-0.35	14.18	-0.12	0.15	-0.25	1.02	-0.19
C4-P	-0.21	0.11	0.08	0.14	25.64	-1.08	0.24	-0.05	-0.12	6.83	-0.11	0.12	-0.11	0.34	0.24
R		0.432	0.197	0.622	0.002	0.096	0.407	0.285	0.262	0.004	0.278	0.164	0.272	0.189	0.122
Q		0.550	0.598	0.476	0.440	0.453	0.424	0.453	0.481	0.539	0.406	0.561	0.444	0.456	0.606

Table continued

Atoms	Experimental RDCs	Theoretical Normalized RDCs				
		Conformer				
		AD	AE	AF	AG	AH
C3'-H3'	-4.55	13.34	12.84	2.85	11.60	26.74
C6'-H6'	-4.44	15.08	13.85	3.59	11.99	25.99
C4'-H4'	1.86	52.67	39.92	24.65	28.71	24.88
C5'-H5'	-1.08	-4.33	-3.44	0.89	-3.51	1.73
C2-H2	-7.25	-2.59	-7.86	-4.48	-11.60	-29.51
C6'-P	0.08	0.48	0.39	0.22	0.39	0.28
C4'-P	-0.07	0.17	0.14	0.08	0.11	0.10
C5'-P	-0.04	0.22	0.17	0.10	0.14	0.11
C1'-P	0.00	1.05	0.89	0.60	0.83	0.81
C1-P	0.86	-0.10	-0.11	-0.32	0.10	0.41
C2-P	0.21	0.09	0.06	0.25	0.66	0.30
C5-P	-0.29	0.36	0.96	0.29	0.31	0.10
C4-P	-0.21	0.18	0.32	0.24	0.34	0.12
R		0.172	0.215	0.373	0.268	0.174
Q		0.431	0.441	0.417	0.457	0.555

3.3. Boltzmann distribution-weight averaged RDC datasets

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 conformer with the lowest energy in the considered ensemble, 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 was considered throughout the work.

All RDC values are given in Hz. The atom numbering used in the tables corresponds to the numbering in Figure 1 of the main text.

Table S40: Boltzmann distribution-weight averaged RDCs of conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-13.11	-28.19	-27.82
C2-H2	31.36	20.83	21.52
C4-H4	0.40	-8.96	-7.32
C6-H6	15.42	16.39	15.82
C1-C8	-0.57	1.02	1.03
C4'-P	-0.04	-0.14	-0.15
C1'-P	-1.21	-2.38	-2.43
C1-P	1.28	-0.63	-0.61
C6-P	0.70	-0.41	-0.42
C8-P	-0.38	-0.03	-0.03
R		0.899	0.911

Table S41: Boltzmann distribution-weight averaged RDCs of conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.03	-45.59	-45.55
C2-H2	35.55	33.69	35.24
C4-H4	-11.31	-14.49	-11.98
C6-H6	15.88	26.50	25.90
C1-C8	-1.96	1.65	1.68
C4'-P	-0.25	-0.23	-0.24
C1'-P	0.41	-3.85	-3.98
C1-P	1.30	-1.02	-1.01
C6-P	0.66	-0.66	-0.69
C5-P	-0.39	-0.43	-0.44
R		0.596	0.596

Table S42: Boltzmann distribution-weight averaged RDCs of conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-17.64	-34.61	-34.16
C2-H2	39.33	25.58	26.43
C4-H4	1.26	-11.00	-8.99
C6-H6	15.89	20.12	19.42
C1-C8	-0.8	1.25	1.26
C4'-P	-0.34	-0.18	-0.18
C8-P	-0.63	-0.04	-0.04
R		0.897	0.909

Table S43: Boltzmann distribution-weight averaged RDCs of conformers of **1-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.99	-43.59	-44.13
C2-H2	34.54	32.21	34.14
C4-H4	-13.18	-13.86	-11.61
C6-H6	14.43	25.34	25.09
C1-C8	-2.15	1.57	1.63
R		0.586	0.578

Table S44: Boltzmann distribution-weight averaged RDCs of conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-13.11	-10.65	-10.66
C2-H2	31.36	36.13	36.45
C4-H4	0.40	-0.18	1.56
C6-H6	15.42	7.41	7.11
C1-C8	-0.57	0.69	0.70
C4'-P	-0.04	-0.05	-0.05
C1'-P	-1.21	-0.78	-0.80
C1-P	1.28	-1.38	-1.33
C6-P	0.70	-0.94	-0.92
C8-P	-0.38	-0.39	-0.39
R		0.962	0.959

Table S45: Boltzmann distribution-weight averaged RDCs of conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.03	-13.33	-13.55
C2-H2	35.55	45.19	46.31
C4-H4	-11.31	-0.23	1.98
C6-H6	15.88	9.27	9.03
C1-C8	-1.96	0.87	0.89
C4'-P	-0.25	-0.07	-0.07
C1'-P	0.41	-0.98	-1.02
C1-P	1.30	-1.73	-1.69
C6-P	0.66	-1.17	-1.18
C5-P	-0.39	-0.27	-0.28
R		0.827	0.809

Table S46: Boltzmann distribution-weight averaged RDCs of conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-17.64	-13.14	-13.17
C2-H2	39.33	44.56	45.01
C4-H4	1.26	-0.22	1.93
C6-H6	15.89	9.14	8.78
C1-C8	-0.8	0.86	0.86
C4'-P	-0.34	-0.06	-0.07
C8-P	-0.63	-0.48	-0.48
R		0.976	0.975

Table S47: Boltzmann distribution-weight averaged RDCs of conformers of **1-SS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.99	-13.92	-14.38
C2-H2	34.54	47.19	49.15
C4-H4	-13.18	-0.24	2.11
C6-H6	14.43	9.68	9.58
C1-C8	-2.15	0.91	0.94
R		0.779	0.756

Table S48: Boltzmann distribution-weight averaged RDCs of conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-13.11	-27.59	-27.28
C2-H2	31.36	21.57	22.19
C4-H4	0.40	-9.16	-7.56
C6-H6	15.42	15.55	14.97
C1-C8	-0.57	0.99	1.01
C4'-P	-0.04	-0.14	-0.14
C1'-P	-1.21	-2.33	-2.36
C1-P	1.28	-0.62	-0.61
C6-P	0.70	-0.40	-0.43
C8-P	-0.38	-0.03	-0.03
R		0.907	0.918

Table S49: Boltzmann distribution-weight averaged RDCs of conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.03	-43.90	-43.99
C2-H2	35.55	34.32	35.77
C4-H4	-11.31	-14.58	-12.19
C6-H6	15.88	24.74	24.14
C1-C8	-1.96	1.58	1.63
C4'-P	-0.25	-0.22	-0.23
C1'-P	0.41	-3.71	-3.81
C1-P	1.30	-0.99	-0.98
C6-P	0.66	-0.63	-0.69
C5-P	-0.39	-0.40	-0.42
R		0.613	0.611

Table S50: Boltzmann distribution-weight averaged RDCs of conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-17.64	-33.85	-33.42
C2-H2	39.33	26.46	27.18
C4-H4	1.26	-11.24	-9.26
C6-H6	15.89	19.07	18.34
C1-C8	-0.8	1.22	1.24
C4'-P	-0.34	-0.17	-0.18
C8-P	-0.63	-0.03	-0.04
R		0.906	0.917

Table S51: Boltzmann distribution-weight averaged RDCs of conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.99	-41.79	-42.40
C2-H2	34.54	32.67	34.48
C4-H4	-13.18	-13.88	-11.75
C6-H6	14.43	23.55	23.27
C1-C8	-2.15	1.50	1.57
R		0.603	0.595

Table S52: Boltzmann distribution-weight averaged RDCs of conformers of **1-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-13.11	-8.93	-9.16
C2-H2	31.36	37.53	37.55
C4-H4	0.40	-0.50	1.72
C6-H6	15.42	6.48	6.49
C1-C8	-0.57	0.67	0.62
C4'-P	-0.04	-0.04	-0.05
C1'-P	-1.21	-0.70	-0.73
C1-P	1.28	-1.38	-1.33
C6-P	0.70	-0.97	-0.95
C8-P	-0.38	-0.39	-0.39
R		0.947	0.947

Table S53: Boltzmann distribution-weight averaged RDCs of conformers of **1-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-SS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.03	-10.78	-11.40
C2-H2	35.55	45.34	46.72
C4-H4	-11.31	-0.60	2.14
C6-H6	15.88	7.82	8.08
C1-C8	-1.96	0.81	0.78
C4'-P	-0.25	-0.05	-0.06
C1'-P	0.41	-0.85	-0.91
C1-P	1.30	-1.67	-1.65
C6-P	0.66	-1.17	-1.18
C5-P	-0.39	-0.28	-0.29
R		0.842	0.820

Table S54: Boltzmann distribution-weight averaged RDCs of conformers of **1-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RS** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-17.64	-11.02	-11.36
C2-H2	39.33	46.35	46.55
C4-H4	1.26	-0.62	2.13
C6-H6	15.89	8.00	8.05
C1-C8	-0.8	0.83	0.77
C4'-P	-0.34	-0.06	-0.06
C8-P	-0.63	-0.48	-0.48
R		0.961	0.964

Table S55: Boltzmann distribution-weight averaged RDCs of conformers of **1-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **1-RR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	7.99	-11.23	-12.09
C2-H2	34.54	47.23	49.52
C4-H4	-13.18	-0.63	2.27
C6-H6	14.43	8.15	8.56
C1-C8	-2.15	0.84	0.82
R		0.799	0.769

Table S56: Boltzmann distribution-weight averaged RDCs of conformers of **2-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **2-SR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-15.10	-20.87	-19.68
C2-H2	-9.75	-0.08	-2.08
C4'-P	0.10	-0.11	-0.10
C1'-P	-1.54	-1.77	-1.71
C1-P	0.46	-0.05	0.03
C2-P	0.17	-0.18	-0.10
C5-P	-0.17	-0.04	-0.01
C3-P	-0.01	-0.14	-0.11
C4-P	-0.09	-0.16	-0.13
R		0.815	0.871

Table S57: Boltzmann distribution-weight averaged RDCs of conformers of **2-SR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **2-RR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-7.34	-23.76	-20.33
C2-H2	-10.16	-0.09	-2.14
C4'-P	-0.02	-0.12	-0.11
C1'-P	-0.75	-2.01	-1.76
C2-P	0.37	-0.20	-0.10
C5-P	-0.34	-0.05	-0.01
C3-P	0.04	-0.16	-0.11
C4-P	-0.23	-0.19	-0.14
R		0.491	0.578

Table S58: Boltzmann distribution-weight averaged RDCs of conformers of **2-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **2-SR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-15.10	-14.00	-13.84
C2-H2	-9.75	-11.89	-12.17
C4'-P	0.10	-0.07	-0.07
C1'-P	-1.54	-1.13	-1.16
C1-P	0.46	0.11	0.16
C2-P	0.17	-0.16	-0.15
C5-P	-0.17	0.12	0.10
C3-P	-0.01	-0.03	-0.03
C4-P	-0.09	0.00	-0.01
R		0.988	0.985

Table S59: Boltzmann distribution-weight averaged RDCs of conformers of **2-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **2-RR** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C4'-H4'	-7.34	-10.00	-9.80
C2-H2	-10.16	-8.49	-8.62
C4'-P	-0.02	-0.05	-0.05
C1'-P	-0.75	-0.81	-0.82
C2-P	0.37	-0.12	-0.10
C5-P	-0.34	0.09	0.07
C3-P	0.04	-0.02	-0.02
C4-P	-0.23	0.00	-0.01
R		0.959	0.964

Table S60: Boltzmann distribution-weight averaged RDCs of conformers of **3-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **3-A** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C3'-H3'	-8.64	-15.36	-17.85
C6'-C6'	-10.03	-14.56	-18.31
C4'-H4'	-13.93	-34.96	-24.60
C5'-H5'	14.56	-12.51	-4.01
C2-H2	-17.16	-27.42	-22.45
C6'-P	-0.16	-0.52	-0.35
C4'-P	-0.21	-0.11	-0.09
C5'-P	-0.02	-0.18	-0.13
C3'P	-0.11	-0.12	-0.11
C1-P	0.87	0.20	0.28
C2-P	0.41	-0.65	-0.30
C5-P	-0.07	-0.02	0.10
C3-P	-0.07	-0.14	-0.05
C4-P	-0.14	-0.10	-0.04
R		0.668	0.802

Table S61: Boltzmann distribution-weight averaged RDCs of conformers of **3-RS** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **3-B** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C3'-H3'	-4.55	-7.86	-7.93
C6'-H6'	-4.44	-7.45	-8.13
C4'-H4'	1.86	-17.89	-10.92
C5'-H5'	-1.08	-6.40	-1.78
C2-H2	-7.25	-14.03	-9.97
C6'-P	0.08	-0.26	-0.15
C4'-P	-0.07	-0.06	-0.04
C5'-P	-0.04	-0.09	-0.06
C1'-P	0.00	-0.40	-0.05
C1-P	0.86	0.10	0.13
C2-P	0.21	-0.33	-0.13
C5-P	-0.29	-0.01	0.04
C4-P	-0.21	-0.05	-0.02
R		0.428	0.590

Table S62: Boltzmann distribution-weight averaged RDCs of conformers of **3-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **3-A** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C3'-H3'	-8.64	-24.75	-21.70
C6'-C6'	-10.03	-23.93	-23.69
C4'-H4'	-13.93	-69.80	-54.38
C5'-H5'	14.56	1.18	6.51
C2-H2	-17.16	23.78	16.78
C6'-P	-0.16	-0.83	-0.61
C4'-P	-0.21	-0.24	-0.19
C5'-P	-0.02	-0.32	-0.25
C3'P	-0.11	-0.29	-0.24
C1-P	0.87	0.08	0.35
C2-P	0.41	-1.04	-0.65
C5-P	-0.07	-1.03	-0.82
C3-P	-0.07	-0.77	-0.59
C4-P	-0.14	-0.77	-0.63
R		0.365	0.453

Table S63: Boltzmann distribution-weight averaged RDCs of conformers of **3-RR** derived from molecular docking before (Unrelaxed) and after (Relaxed) normal mode relaxation; normalized against **3-B** experimental values.

Atoms	Experimental RDCs	Normalized Boltzmann averaged RDCs	
		Unrelaxed	Relaxed
C3'-H3'	-4.55	10.16	15.13
C6'-H6'	-4.44	9.82	16.51
C4'-H4'	1.86	28.65	37.90
C5'-H5'	-1.08	-0.48	-4.53
C2-H2	-7.25	-9.76	-11.70
C6'-P	0.08	0.34	0.43
C4'-P	-0.07	0.10	0.14
C5'-P	-0.04	0.13	0.17
C1'-P	0.00	0.72	0.17
C1-P	0.86	-0.03	-0.24
C2-P	0.21	0.43	0.45
C5-P	-0.29	0.42	0.57
C4-P	-0.21	0.32	0.44
R		0.287	0.209

3.4. Parameters for machine learning-aided (ML) elimination of redundant structures

The mean shift clustering algorithm specifies the cluster size using a so-called bandwidth parameter. The value of this parameter determines whether each data point belongs to a given cluster. This parameter is proportional to the size of a given cluster. The optimal values for each structure were decided by trial and error. In particular, various parameter values were initially used for each molecule. The distribution of dihedral angles of all obtained conformers between resulting clusters was visually examined. The correct parameter value corresponded to the state when the conformers were correctly sorted into clusters, i.e., clusters contained conformers within at most 10° difference between the corresponding dihedral angles.

Table S64: Total number of conformers discovered using molecular docking, number of unique conformers identified via machine learning-aided elimination, value of the bandwidth parameter for each isomer of **2** and **3**.

Molecule →	**2-SR**	**2-RR**	**3-RS**	**3-RR**
Total number of conformers	39	34	102	162
Number of unique conformers	21	21	23	34
Bandwidth parameter	12	5	10	20

4. X-ray diffraction

4.1. X-ray details

The X-ray data for colorless crystals of isomers of **1** were obtained at 150 K using Oxford Cryostream low-temperature device with a Bruker D8-Venture diffractometer equipped with Mo (Mo/K_α radiation; λ = 0.71073 Å) microfocus X-ray (IμS) source, Photon III CMOS detector and Oxford Cryosystems cooling device was used for data collection. Obtained data were treated by XT-version 2019/1 and SHELXL-2019/3 (or higher) software implemented in APEX3 v2019.6-0 (Bruker AXS) system.[2] $R_{int} = \sum \left| F_o^2 - F_{o,mean}^2 \right| / \sum F_o^2$, S = $[\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum \left| \left| F_o \right| - \left| F_c \right| \right| / \sum \left| F_o \right|$ for observed data, $wR(F^2)$ = $[\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data. Crystallographic data for all structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC nos. 2277412–2277415. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EY, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

The frames for all compounds were integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The structures were solved and refined using the Bruker SHELXTL Software Package.

Hydrogen atoms were mostly localized on a difference Fourier map, however, to ensure uniformity of treatment of crystal, all hydrogen atoms except of those involved in H-bonds were recalculated into idealized positions (riding model) and assigned temperature factors $H_{iso}(H)$ = 1.2 U_{eq} (pivot atom) or of 1.5U_{eq} (methyl). H atoms in methyl, methylene moieties and C-H in aromatic rings were placed with C-H distances of 0.96, 0.97 and 0.93 Å. The positional disorders of the phenyl ring in **1-RS** and **1-SR** were treated by standard methods with occupancy ~ 1:1. Friedel fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.[3]

Table S65: Experimental details for **1-SS**

Crystal data	
Chemical formula	$C_{16}H_{21}O_3P$
M_r	292.30
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, *b*, *c* (Å)	9.9495(2), 11.5590(2), 26.1562(5)
V (Å^3)	3008.13(10)
Z	8
Radiation type	Mo*K*α
μ (mm^{-1})	0.19
Crystal size (mm)	0.59 × 0.44 × 0.37
Data collection	
Diffractometer	Bruker D8 - Venture
Absorption correction	Multi-scan
T_{min}, T_{max}	0.669, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	64670, 7451, 7235
R_{int}	0.036
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.069, 1.07
No. of reflections	7451
No. of parameters	367
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.21
Absolute structure	Flack x determined using 3121 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.001(12)

Computer programs: Bruker Instrument Service vV6.2.3, *APEX4* v2021.4-1 (Bruker AXS), *SAINT* V8.40B (Bruker AXS Inc., 2019), *SHELXT* 2018/2 (Sheldrick, 2014), *SHELXL2019*/1 (Sheldrick, 2019), Bruker *SHELXTL*.

Table S66: Experimental details for **1-RR**

Crystal data	
Chemical formula	$C_{16}H_{21}O_3P$
M_r	292.30
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, *b*, *c* (Å)	9.9615(6), 11.5646(7), 26.2104(14)
V (Å^3)	3019.5(3)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.19
Crystal size (mm)	0.25 × 0.20 × 0.16
Data collection	
Diffractometer	Bruker D8 - Venture
Absorption correction	Multi-scan *SADABS2016*/2 - Bruker AXS area detector scaling and absorption correction
T_{min}, T_{max}	0.603, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	45757, 7542, 7145
R_{int}	0.058
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.670
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.037, 0.096, 1.07
No. of reflections	7542
No. of parameters	367
No. of restraints	350
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, –0.26
Absolute structure	Flack x determined using 2958 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.04(3)

Computer programs: Bruker Instrument Service vV6.2.3, *APEX4* v2021.4-1 (Bruker AXS), *SAINT* V8.40B (Bruker AXS Inc., 2019), *SHELXT* 2018/2 (Sheldrick, 2014), *SHELXL2019*/1 (Sheldrick, 2019), Bruker *SHELXTL*.

Table S67: Experimental details for **1-RS**

Crystal data	
Chemical formula	$C_{16}H_{21}O_3P$
M_r	292.30
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	150
a, *b*, *c* (Å)	10.2898(10), 6.9020(6), 11.6872(9)
β (°)	114.772(3)
V (Å^3)	753.65(12)
Z	2
Radiation type	Mo*K*α
μ (mm^{-1})	0.19
Crystal size (mm)	0.22 × 0.18 × 0.13
Data collection	
Diffractometer	Bruker D8 - Venture
Absorption correction	Multi-scan *SADABS2016*/2 - Bruker AXS area detector scaling and absorption correction
T_{min}, T_{max}	0.643, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29459, 2874, 2709
R_{int}	0.066
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.613
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.101, 1.09
No. of reflections	2874
No. of parameters	179
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.26
Absolute structure	Flack x determined using 1197 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.01(3)

Computer programs: Bruker Instrument Service vV6.2.3, *APEX4* v2021.4-1 (Bruker AXS), *SAINT* V8.40B (Bruker AXS Inc., 2019), *SHELXT* 2018/2 (Sheldrick, 2014), *SHELXL2019*/1 (Sheldrick, 2019), Bruker *SHELXTL*.

Table S68: Experimental details for **1-SR**

Crystal data	
Chemical formula	$C_{16}H_{21}O_3P$
M_r	292.30
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	150
a, *b*, *c* (Å)	10.2826(3), 6.9016(2), 11.6832(3)
β (°)	114.723(1)
V (Å^3)	753.12(4)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.19
Crystal size (mm)	0.56 × 0.51 × 0.32
Data collection	
Diffractometer	Bruker D8 - Venture
Absorption correction	Multi-scan
T_{min}, T_{max}	0.696, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13391, 2698, 2664
R_{int}	0.026
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.085, 1.07
No. of reflections	2698
No. of parameters	149
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.24
Absolute structure	Flack x determined using 1180 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−0.03(2)

Computer programs: Bruker Instrument Service vV6.2.3, *APEX4* v2021.4-1 (Bruker AXS), *SAINT* V8.40B (Bruker AXS Inc., 2019), *SHELXT* 2018/2 (Sheldrick, 2014), *SHELXL2019*/1 (Sheldrick, 2019), Bruker *SHELXTL*.

4.2. Crystallography

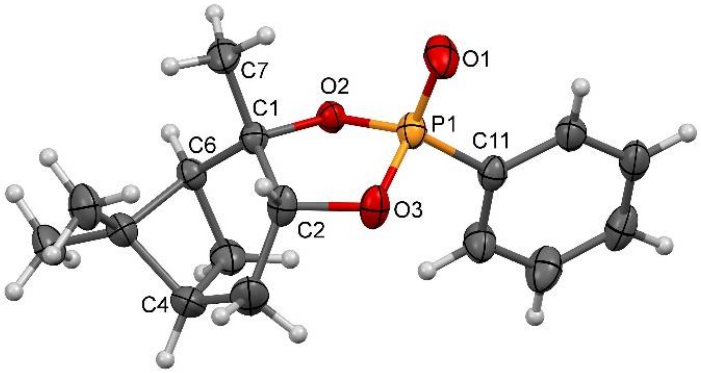


Figure S1: The molecular structure of **1-SS**, ORTEP view 50% probability level, one of two independent molecules is omitted for clarity.

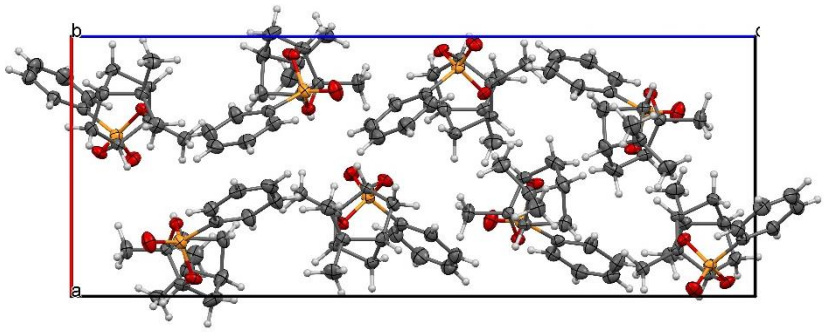


Figure S2: The crystal packing view (along the b-axis) within the structure of **1-SS** – ORTEP view 50% probability level.

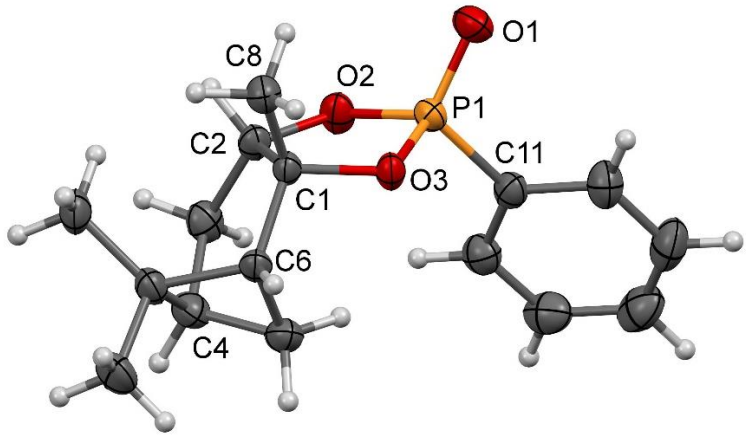


Figure S3: The molecular structure of **1-RR** ORTEP view 50% probability level, one of two independent molecules is omitted for clarity.

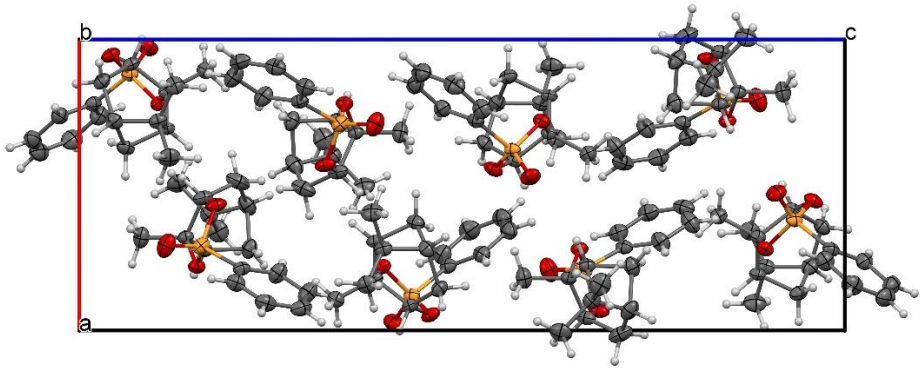


Figure S4: The crystal packing view (along the b-axis) within the structure of **1-RR** – ORTEP view 50% probability level.

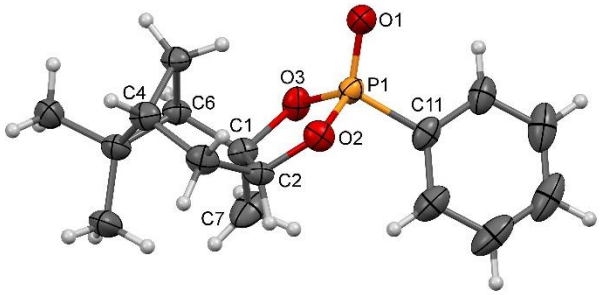


Figure S5: The molecular structure of **1-RS**, ORTEP view 50% probability level, one of two positions of the disordered phenyl ring is omitted for clarity.

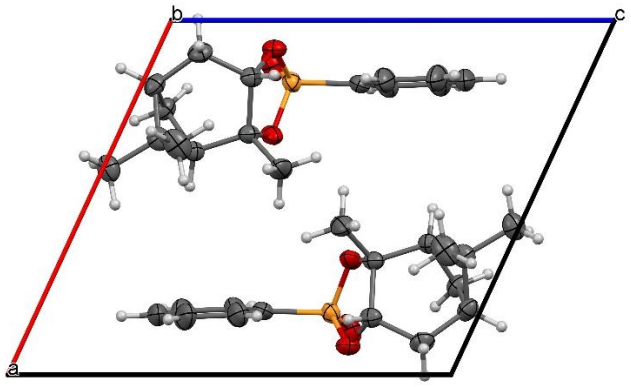


Figure S6: The crystal packing view (along the b-axis) within the structure of **1-RS** – ORTEP view 50% probability level.

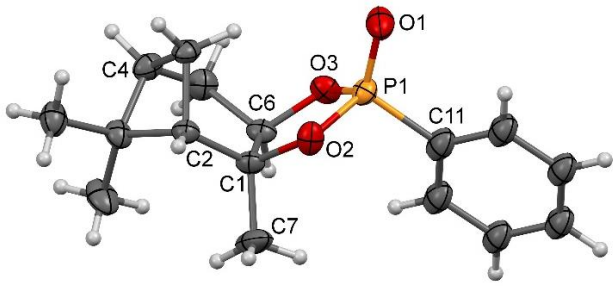


Figure S7: The molecular structure of **1-SR**, ORTEP view 50% probability level, one of two positions of the disordered phenyl ring is omitted for clarity.

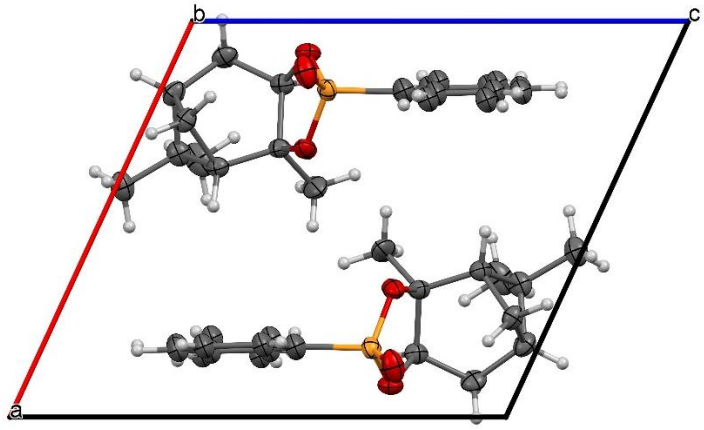


Figure S8: The crystal packing view (along the b-axis) within the structure of **1-SR** – ORTEP view 50% probability level.

All structures determined by crystallographic techniques reveal usual bonding and geometrical parameters for phenylphosphonates. All crystallize in chiral space groups (monoclinic $P2_1$ or orthorhombic $P2_12_12_1$), where the only one isomer is found in each case. Flack parameters for evaluation of the absolute configuration of all determined and refined structures gave very good results and the configuration at the carbon centers are in perfect match with configuration known from the synthesis of starting material.

Surprisingly enough, the only reported compound, which could be directly compared to studied species is 2,4,5-triphenyl-1,3,2-dioxaphospholane 2-oxide[4]. Although the similarities in bond distances and angles in this phospholane-2-oxide and all on newly prepared species are negligible, the literature example exhibits

significant deviation of the phospholane-2-oxide ring from planarity, a common feature of our compound's structures.

5. Compound characterization: NMR spectra

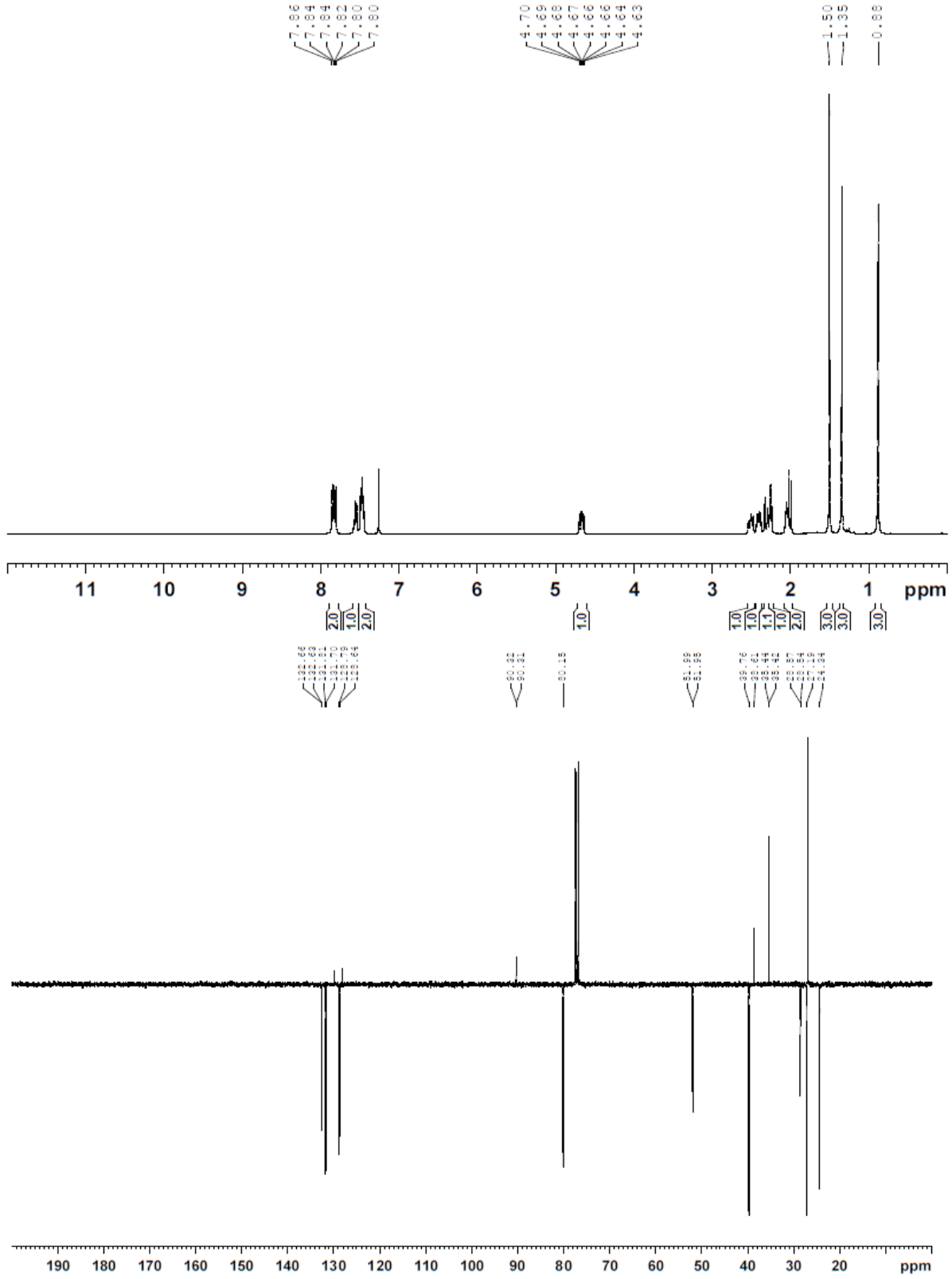


Figure S9: ^{1}H (top) and ^{13}C APT (bottom) NMR spectra of **1-SR** in $CDCl_3$ measured at room temperature.

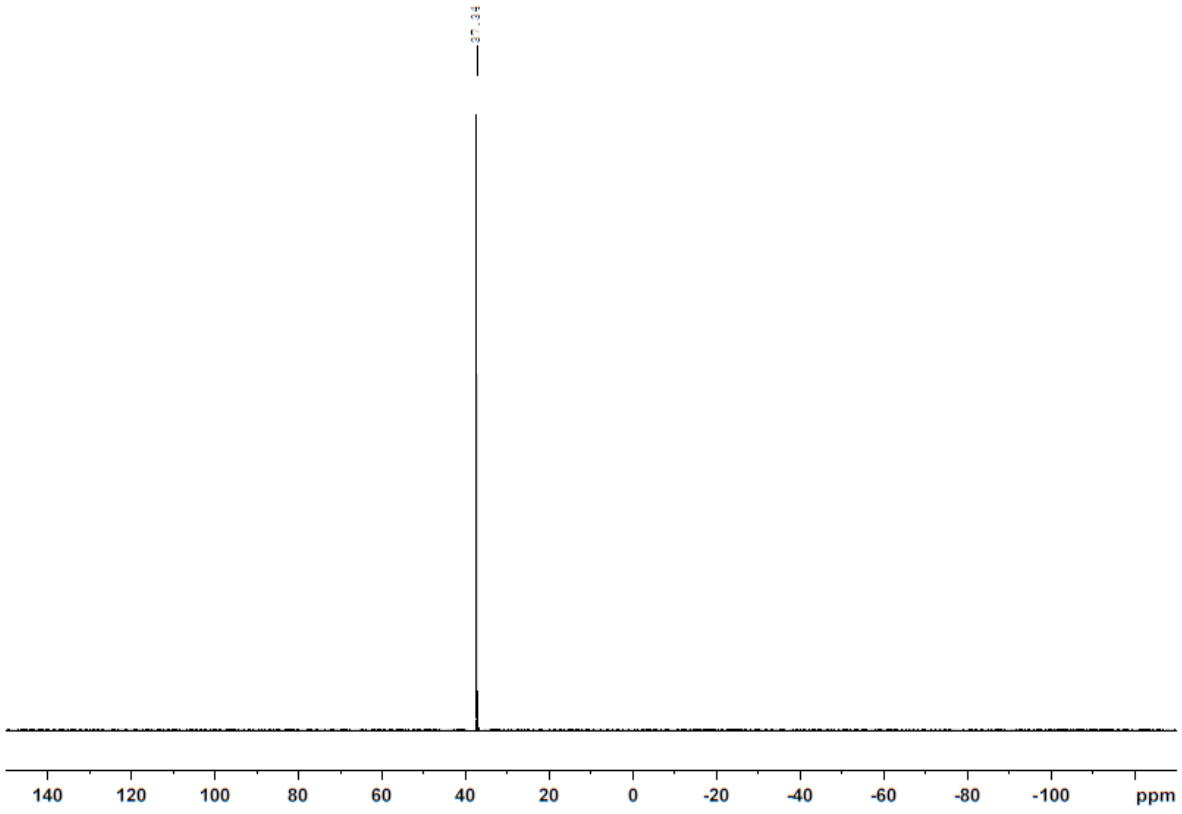


Figure S10: ^{31}P NMR spectra of **1-SR** in $CDCl_3$ measured at room temperature.

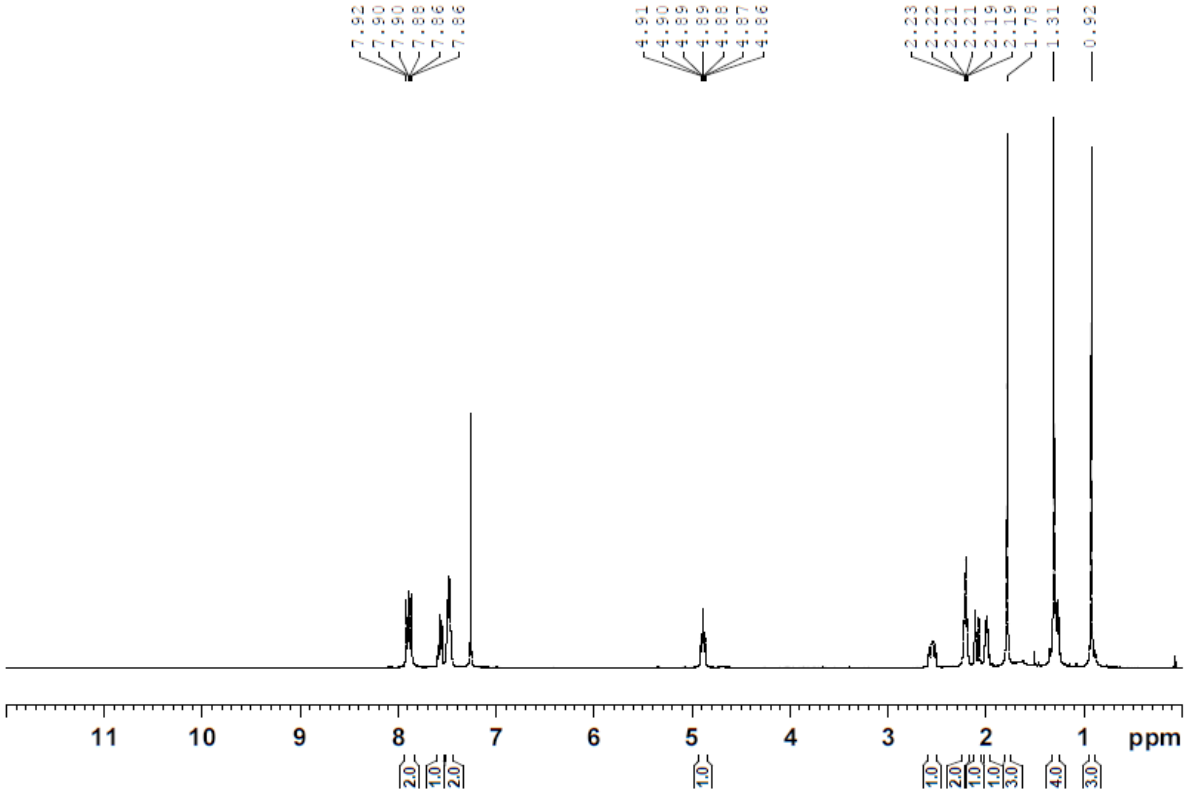


Figure S11: ^{1}H NMR spectra of **1-SS** in $CDCl_3$ measured at room temperature.

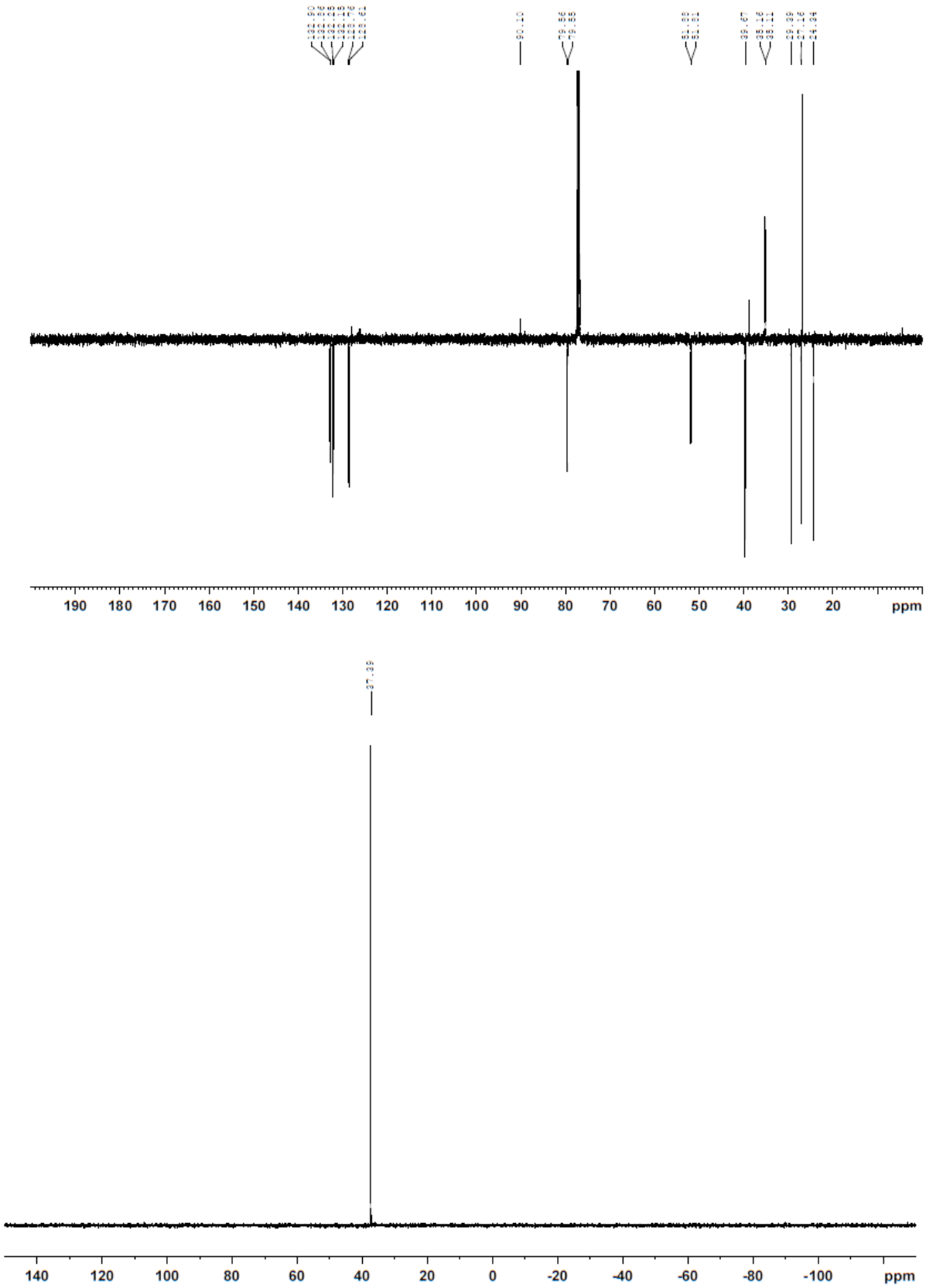


Figure S12: ^{13}C APT (top) and ^{31}P (bottom) NMR spectra of **1-SS** in $CDCl_3$ measured at room temperature.

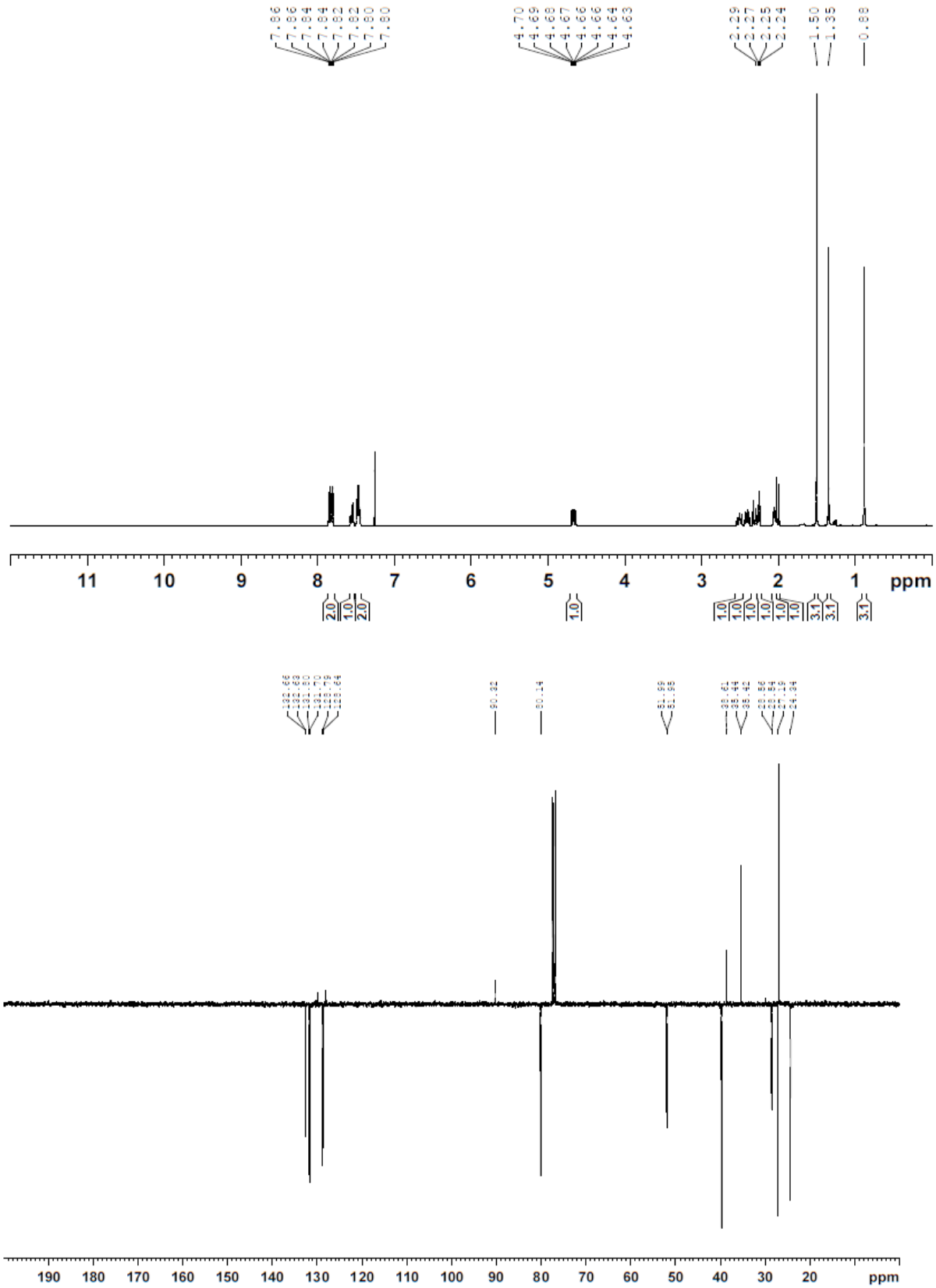


Figure S13: ^{1}H (top) and ^{13}C APT (bottom) NMR spectra of **1-RS** in $CDCl_3$ measured at room temperature.

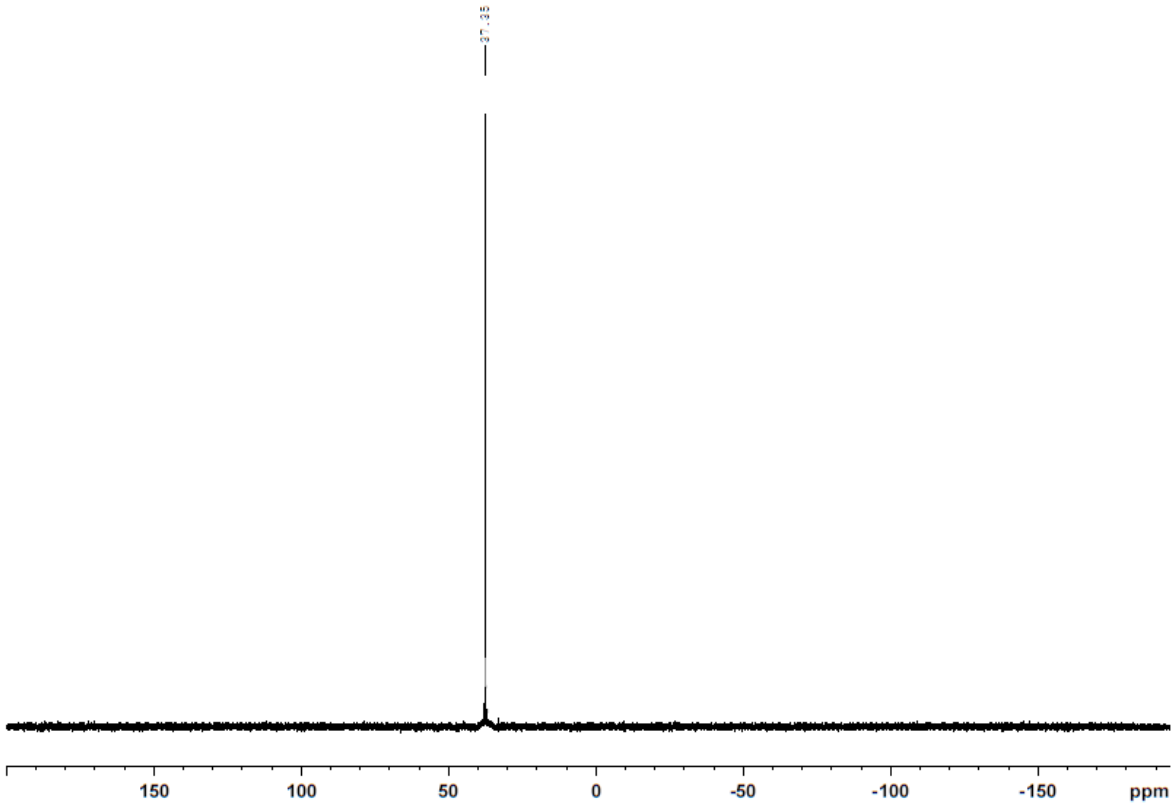


Figure S14: ^{31}P NMR spectra of **1-RS** in $CDCl_3$ measured at room temperature.

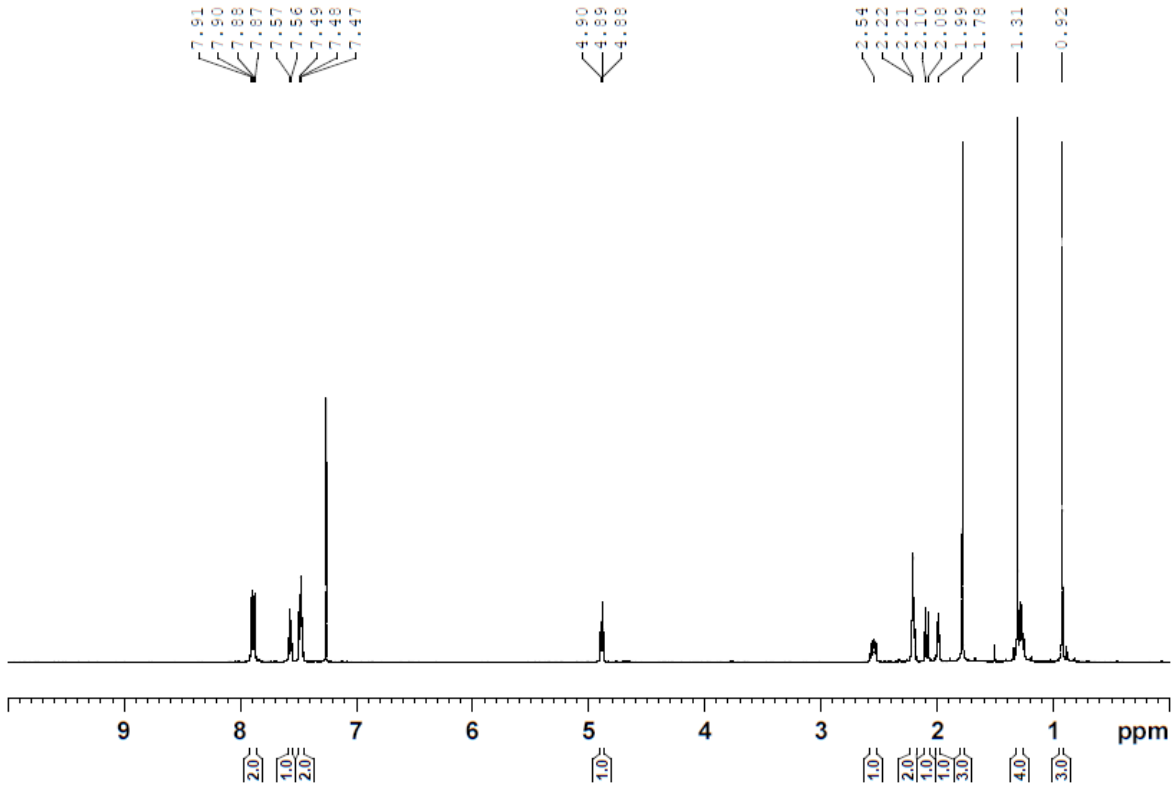


Figure S15: ^{1}H NMR spectra of **1-RR** in $CDCl_3$ measured at room temperature.

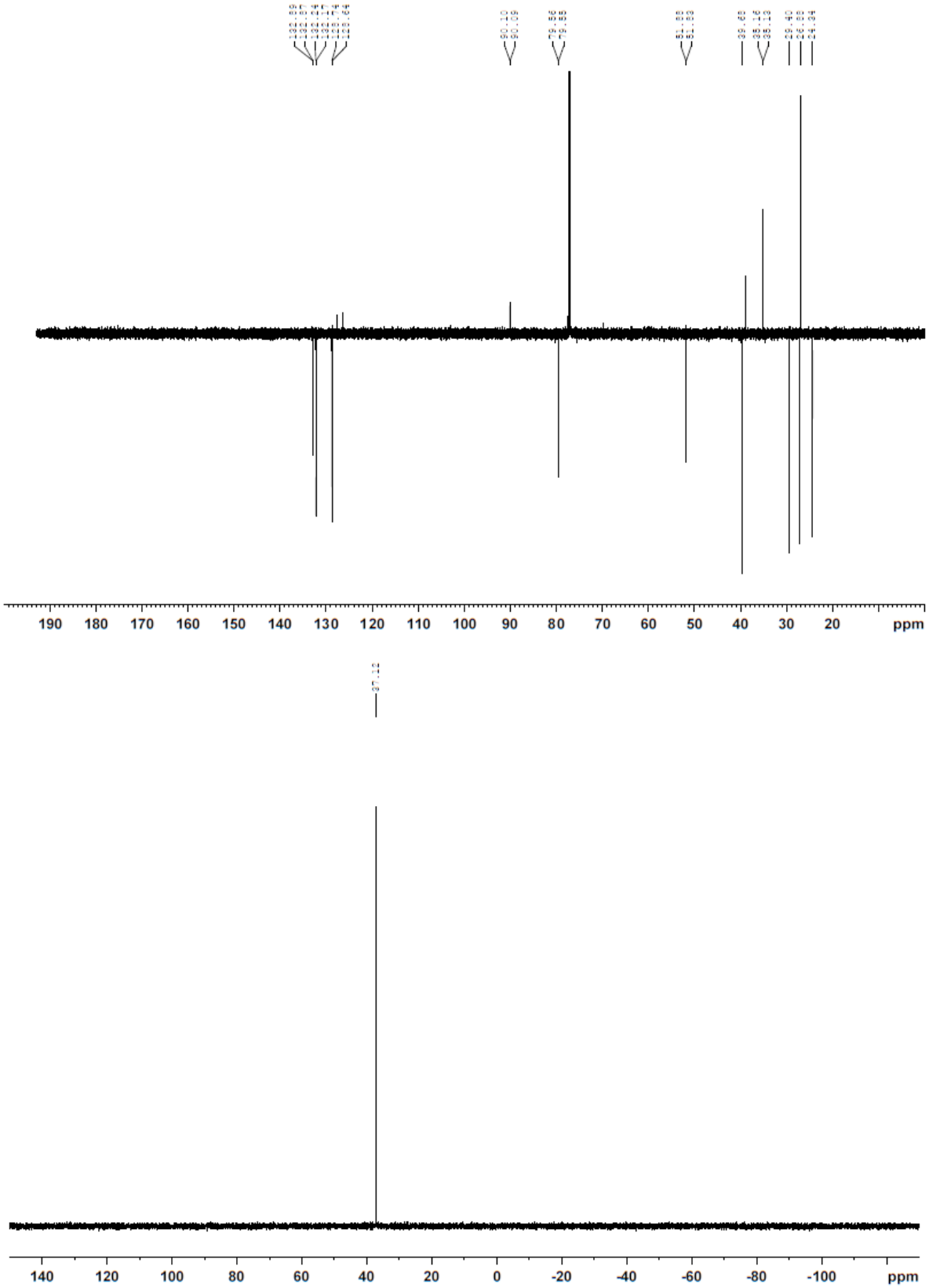


Figure S16: ^{13}C APT (top) and ^{31}P (bottom) NMR spectra of **1-RR** in $CDCl_3$ measured at room temperature.

6. Compound characterization: HR-MS spectra

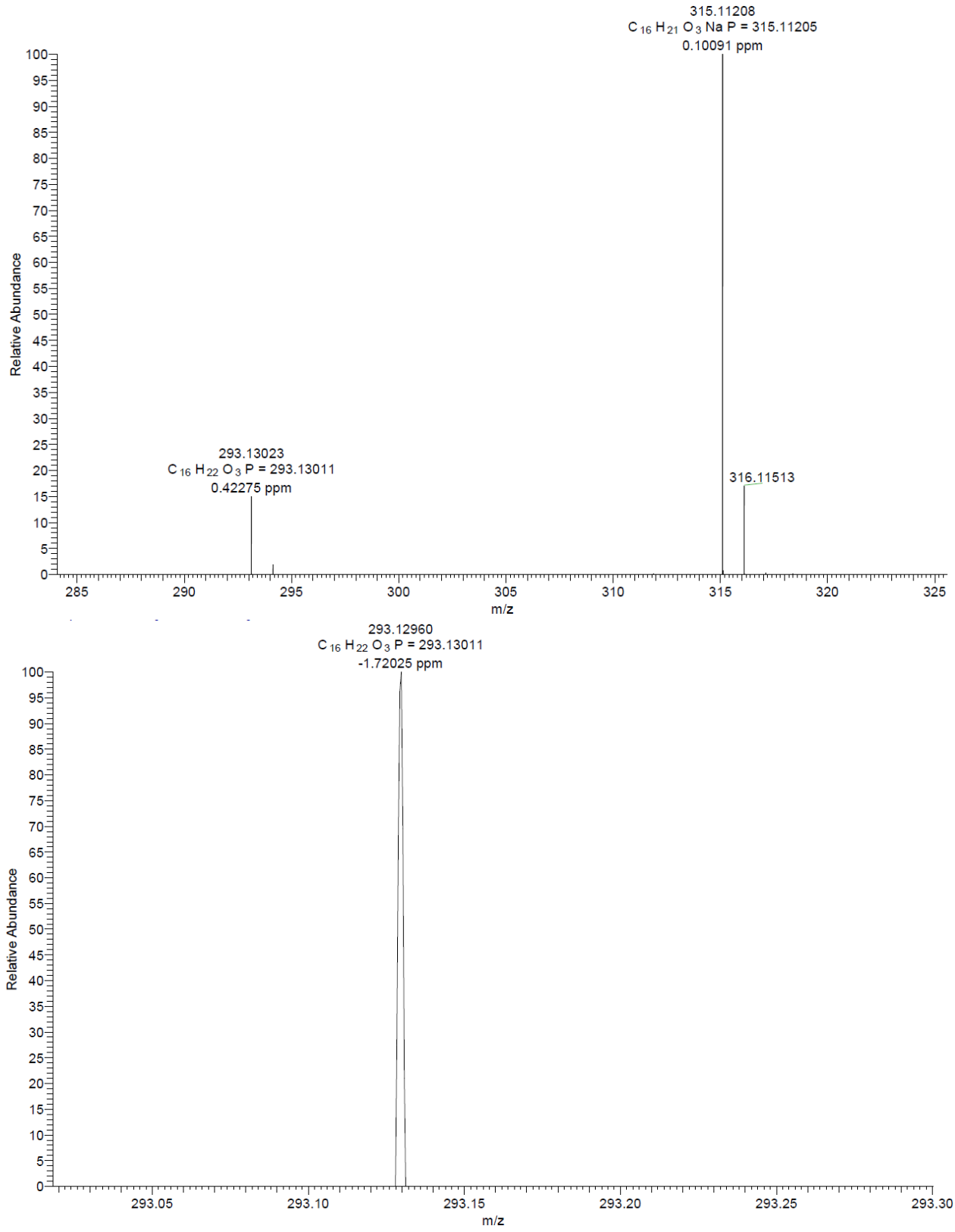


Figure S17: HR-MS spectra of **1-SR** (top) and **1-SS** (bottom).

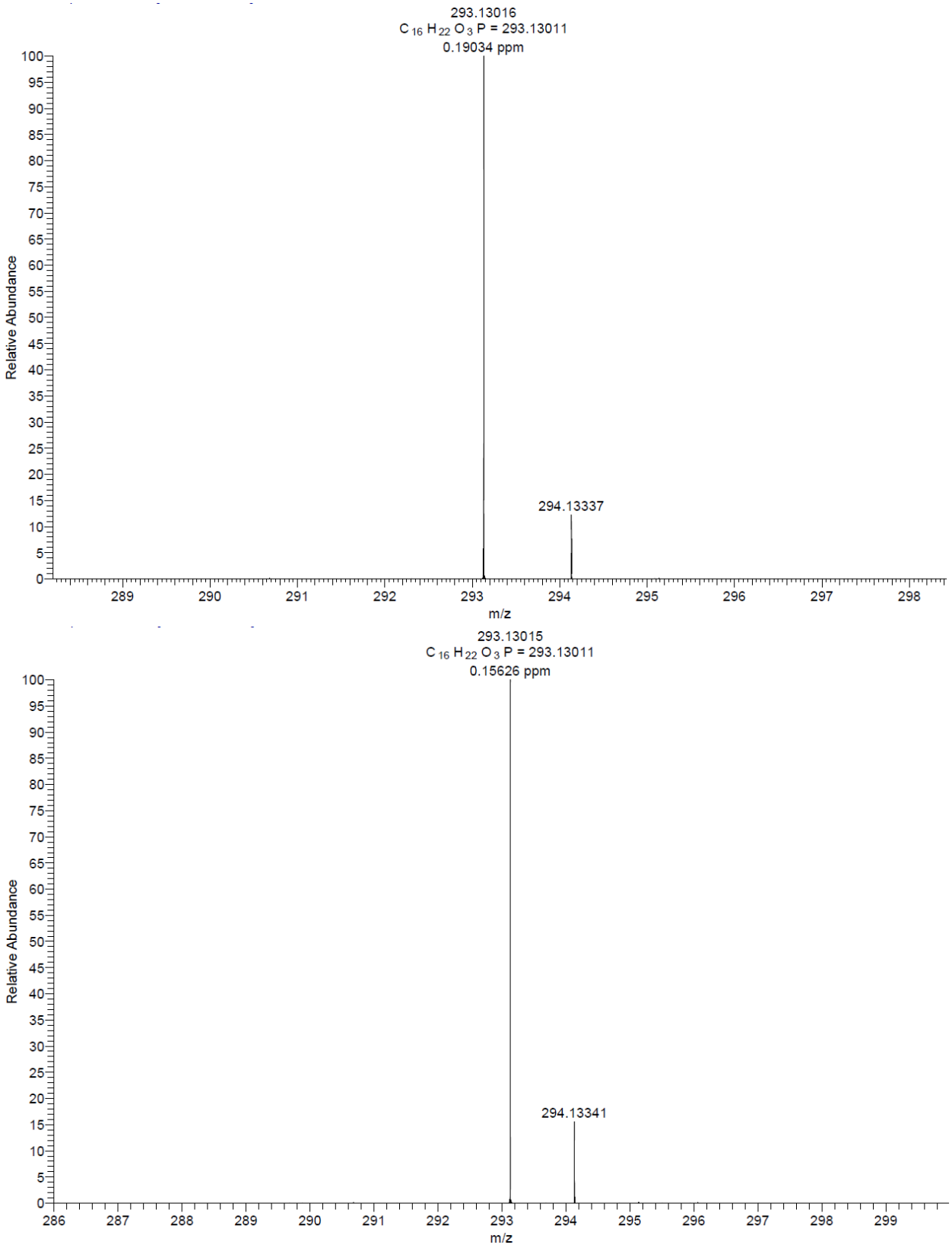


Figure S18: HR-MS spectra of **1-RS** (top) and **1-RR** (bottom).

7. References

1. X. Tian, T. A. Karl, S. Reiter, S. Yakubov, R. de Vivie-Riedle, B. König and J. P. Barham, *Angew. Chem. Int. Ed.*, 2021, **60**, 20817-20825.
2. G. Sheldrick, *Acta Crystallogr. A*, 2015, **71**, 3-8.
3. S. Parsons, H. Flack and T. Wagner, *Acta Crystallogr. B: Struct. Sci. Cryst. Eng. Mater.*, 2013, **69**, 249-259.
4. D. Cordes, G. Hua, A. Slawin and D. Woollins, *Acta Crystallogr. E*, 2011, **67**, o1790.