Electronic Supplementary Information

Substituent Effects in the Crystallization of Zr-Hydroxamate Metal−Organic Frameworks

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1. General procedures

All purchased chemicals were used without further purification except where otherwise noted. Ultrapure water was obtained from a Millipak® Express 40 system (Merk-Millipore, Darmstadt, Germany).

Powder X-ray diffraction (PXRD) patterns were collected on a Rigaku MiniFlex600 at 40 kV, 40 mA for Cu Kα, (λ = 1.54178 Å) with a scan speed of 20°/min from 3° to 50° at a step size of 0.01°. The simulated powder pattern was obtained using Materials Studio based on the crystal structure of the corresponding MOF.

Single-crystal X-ray diffraction (SC-XRD) data for SUM-1-F, SUM-1-Cl and SUM-1-Br were collected on a Bruker D8 Venture diffractometer under the following conditions: SUM-1-F at 200 K using Cu Kα radiation (λ = 1.54178 Å), SUM-1-Cl at 100 K using Cu Kα radiation (λ = 1.54178 Å) and SUM-1-Br at 237 K using Mo Kα radiation (λ = 0.71073 Å).

The crystal structures were solved with direct method using SHELXT[1] and refined by full-matrix least-squares on F^2 using SHELXL2 in Olex2.[3] All non-H atoms were located easily and refined anisotropically. Idealized atom positions were calculated for H atoms.

^{1}H NMR spectra were collected on a JNM-ECZ400S/L1 (400 MHz) spectrometer (JEOL Ltd., Tokyo, Japan).

Optical microscopic images were obtained using a Ruihong BM-500T microscope.

N_2 adsorption–desorption isotherms were collected on a BELSORP MAX system (MicrotracBEL, Japan). CO_2 adsorption–desorption isotherms were collected on a Quantachrome Quadrasorb-EvO.

Thermogravimetric analysis (TGA) was carried out on a TA Discovery SDT 650 simultaneous thermal analyzer from room temperature to 800 ℃ at a heating rate of 10 ℃/min in a N_2 flow of 100 mL/min.

2. Synthesis of ligands and MOFs

2.1 Synthesis of 2,5-difluoro-1,4-benzenedihydroxamic acid (H_2-F_2-BDHA)[4]

Fig. S1 Synthetic route of H_2-F_2-BDHA.

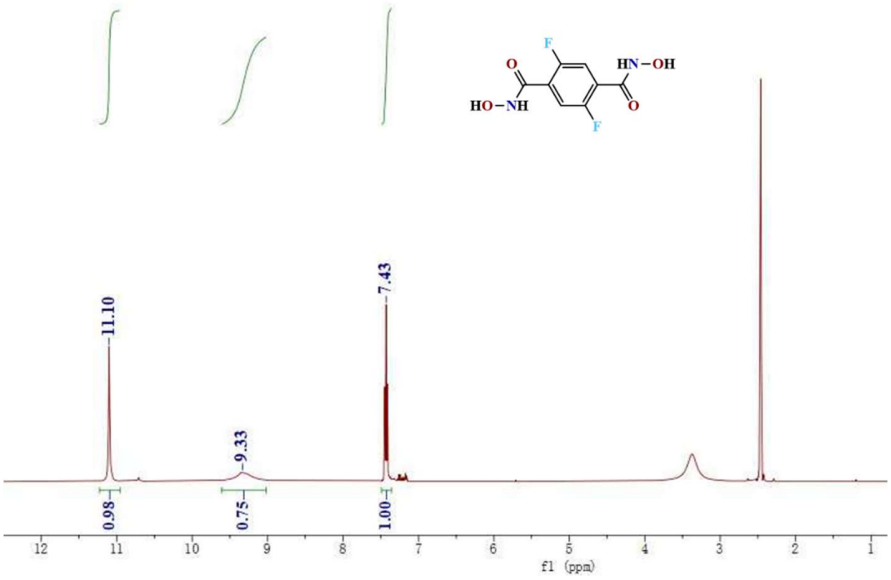

Fig. S2 ^{1}H NMR spectrum of H_2-F_2-BDHA in DMSO-d_6.

2.2 Synthesis of 2,5-dichloro-1,4-benzenedihydroxamic acid (H_2-Cl_2-BDHA)[4]

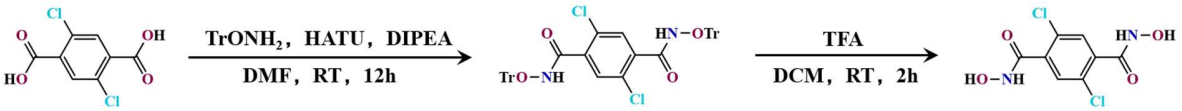

Fig. S3 Synthetic route of H_2-Cl_2-BDHA.

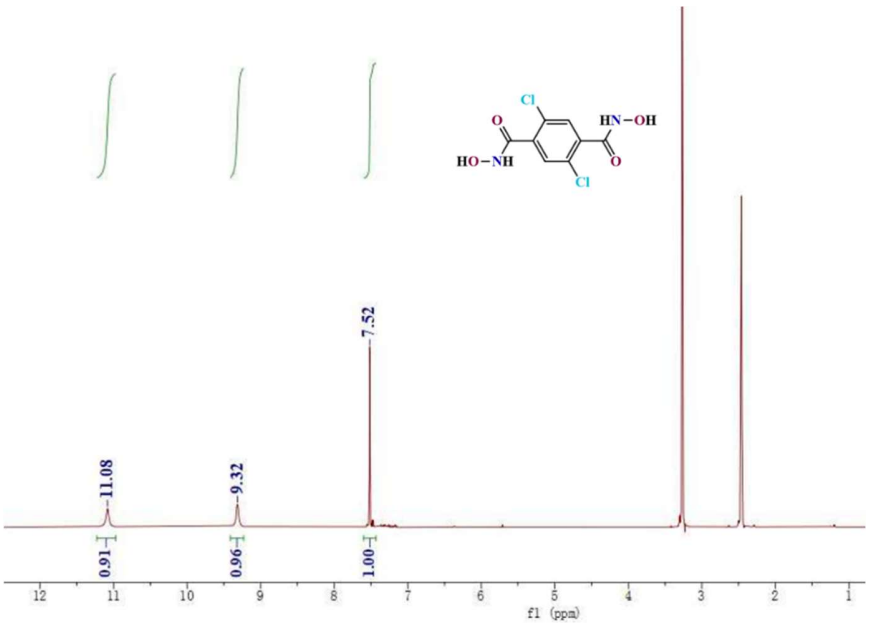

Fig. S4 ^{1}H NMR spectrum of H_2-Cl_2-BDHA in DMSO-d_6.

2.3 Synthesis of 2,5-dibromo-1,4-benzenedihydroxamic acid (H_2-Br_2-BDHA)[4]

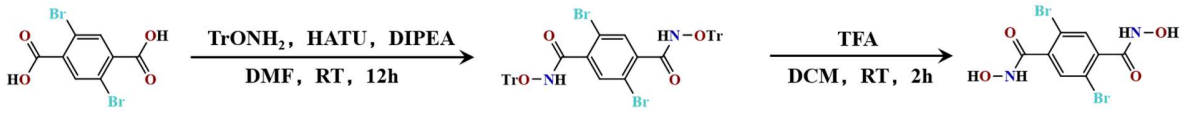

Fig. S5 Synthetic route of H_2-Br_2-BDHA.

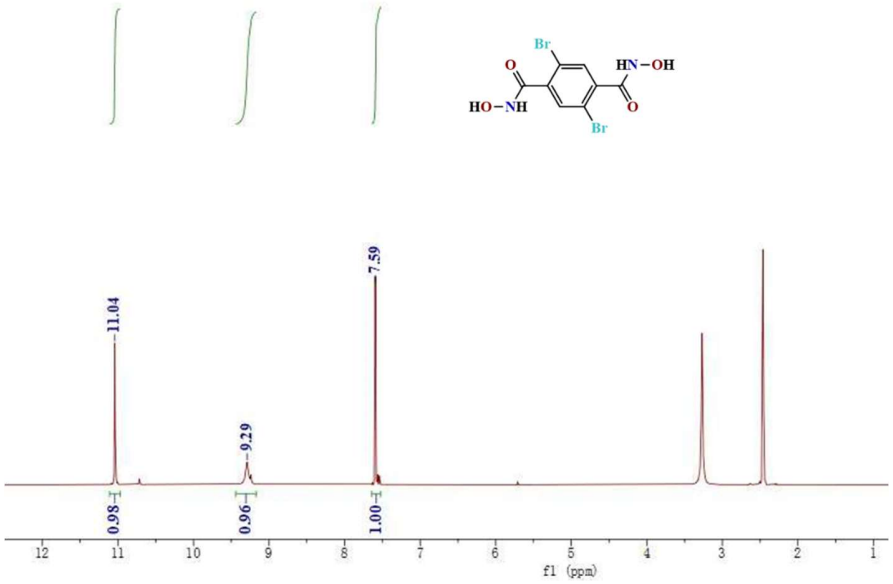

Fig. S6 ^{1}H NMR spectrum of H_2-Br_2-BDHA in DMSO-d_6.

2.4 Synthesis of SUM-1-pz

SUM-1-pz was synthesized according to the procedure reported by Shao et al[5]. Ultrasonic dissolve pyrazine-2,5-dihyroxamic acid (PZDH) (5.9 mg, 0.030 mmol) and $ZrCl_4$ (1.17 mg, 0.005 mmol) in 1 mL DMF in a 4 mL glass bottle. Then add 250 μL HCl and keep the mixture at 90 °C for 72 h. After cooling to room temperature, collect the single crystals. Before drying in the air, wash the crystals with dry DMF (3 × 20 mL) and then with acetone (3 × 20 mL).

2.5 Synthesis of SUM-1-F

Dissolve H_2-F_2-BDHA (13.9 mg, 0.06 mmol) and $ZrCl_4$ (2.3 mg, 0.01 mmol) in 1 mL DMF in a 4 mL glass bottle. Then add 400 μL HCl and keep the mixture at 120 °C for 24 h. After cooling to room temperature, collect the single crystals. Before drying in the air, wash the crystals with dry DMF (3 × 20 mL) and then with acetone (3 × 20 mL).

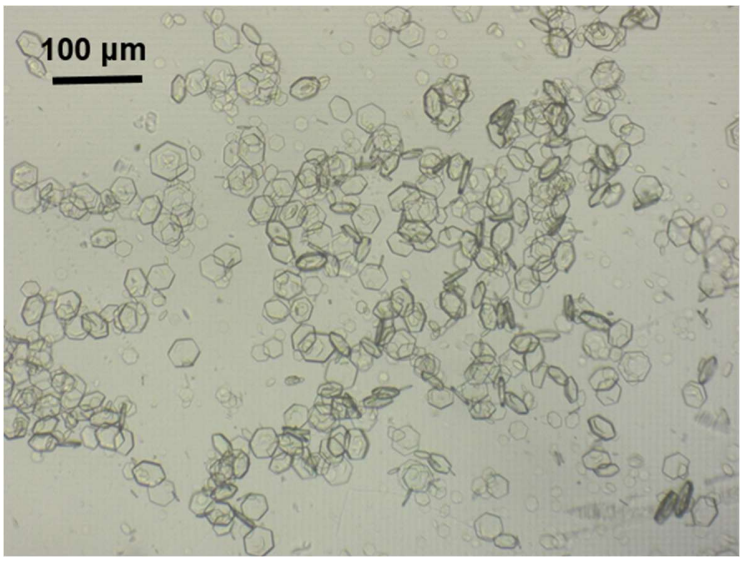

Fig. S7 Optical image of SUM-1-F Crystals.

2.6 Synthesis of SUM-1-Cl

Dissolve H_2-Cl_2-BDHA (21.2 mg, 0.08 mmol) and $ZrCl_4$ (2.3 mg, 0.01 mmol) in 1 mL DMF in a 4 mL glass bottle. Then add 400 μL HCl, 700 μL H_2O and keep the mixture at 120 °C for 24 h. After cooling to room temperature, collect the single crystals. Before drying in the air, wash the crystals with dry DMF (3 × 20 mL) and then with acetone (3 ×

20 mL).

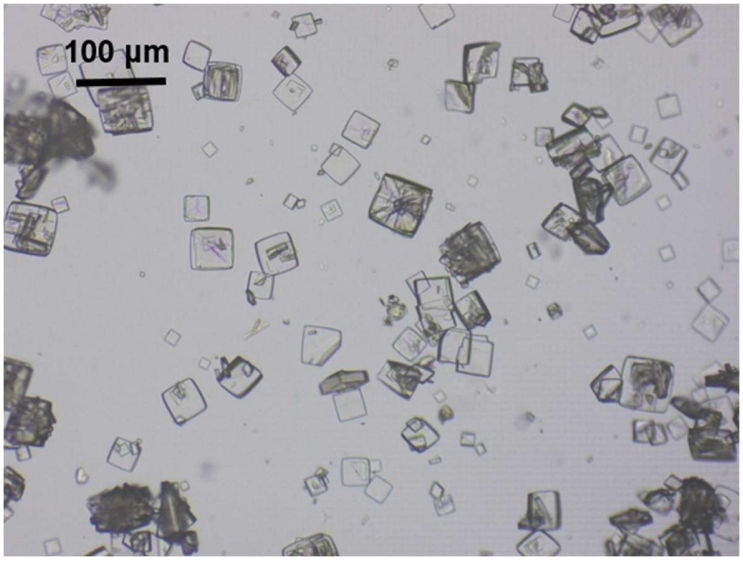

Fig. S8 Optical image of SUM-1-Cl Crystals.

2.7 Synthesis of SUM-1-Br

Dissolve H_2-Br_2-BDHA (21.2 mg, 0.06 mmol) and $ZrCl_4$ (2.3 mg, 0.01 mmol) in 1 mL DMF in a 4 mL glass bottle. Then add 400 μL HCl, 600 μL H_2O and keep the mixture at 120 °C for 24 h. After cooling to room temperature, collect the single crystals. Before drying in the air, wash the crystals with dry DMF (3 × 20 mL) and then with acetone (3 × 20 mL).

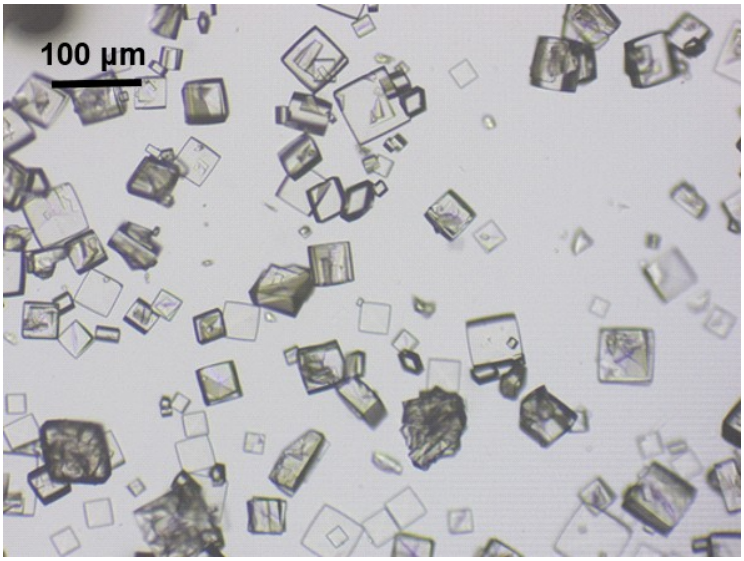

Fig. S9 Optical image of SUM-1-Br Crystals.

3. Crystal structures of SUM-1-F, SUM-1-Cl and SUM-1-Br

3.1 Crystal structure of SUM-1-F

Table S1 Crystal data and structure refinement details for SUM-1-F.

CCDC deposition number	2528071
Compound name	SUM-1-F
Formula	$C_{20}H_{24}Cl_2F_4N_6O_8Zr$
Formula weight	714.57
Temperature/K	200.00
Crystal system	trigonal
Space group	$P\bar{3}c1$
a/Å	23.2456(12)
b/Å	23.2456(12)
c/Å	16.2338(11)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	7596.8(9)
Z	6
ρ_{calc} g/cm^3	0.937
μ/mm^{-1}	3.164
F(000)	2160.0
Crystal size/mm^3	0.13 × 0.11 × 0.09
Radiation	CuKα (λ = 1.54178)
Theta range for data collection /°	7.606 to 149.762
Index ranges	-26 ≤ h ≤ 29, -29 ≤ k ≤ 28, -20 ≤ l ≤ 17
Reflections collected	46976
Independent reflections	5196 [R_{int} = 0.1202, R_{sigma} = 0.0514]
Data / restraints / parameters	5196/75/218
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0466, wR_2 = 0.1313
R indices (all data)	R_1 = 0.0559, wR_2 = 0.1372
Largest diff. peak and hole /e Å^{-3}	0.45/-1.02

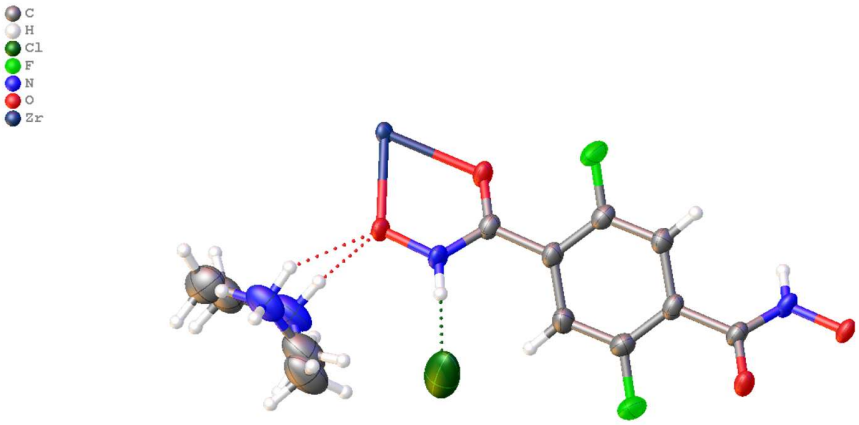

Fig. S10 ORTEP diagram of the asymmetric unit of SUM-1-F (50% probability factor for the thermal ellipsoids), generated in Olex2-1.5.

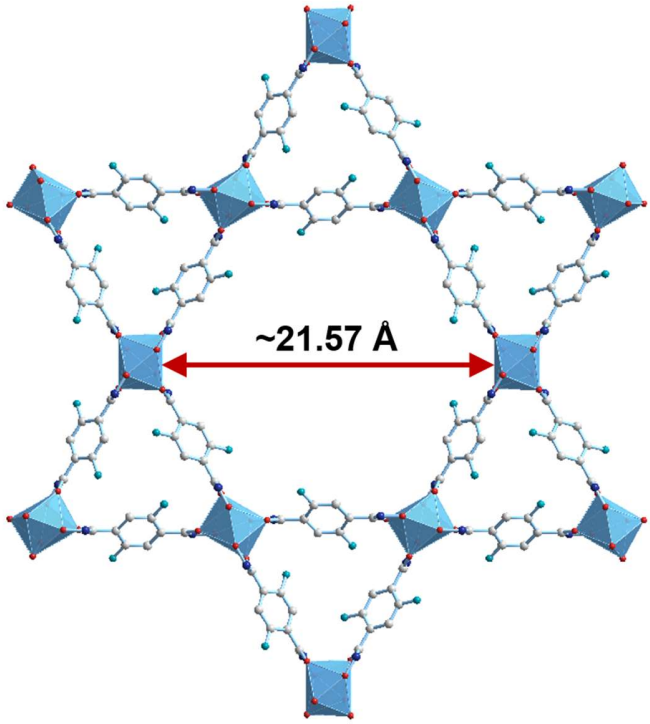

Fig. S11 Crystal structure of SUM-1-F, viewed along the *c* axis. Zr: blue polyhedra; C: white spheres; N: dark blue spheres; O: red spheres; F: teal spheres; H: omitted for clarity.

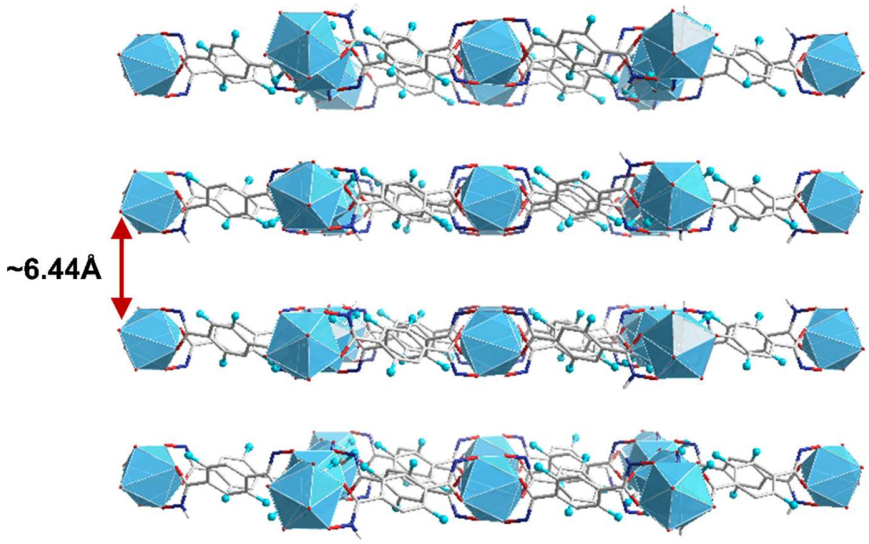

Fig. S12 Crystal structure of SUM-1-F, in packed mode, viewed along the *b* axis. Zr: blue polyhedra; C: white spheres; N: dark blue spheres; O: red spheres; F: teal spheres; H: omitted for clarity.

3.2 Crystal structure of SUM-1-Cl

Table S2 Crystal data and structure refinement details for SUM-1-Cl.

CCDC deposition number	2528072
Compound name	SUM-1-Cl
Formula	$C_{22}H_{22}Cl_6N_6O_{10}Zr$
Formula weight	834.37
Temperature/K	100.00
Crystal system	orthorhombic
Space group	*Ibam*
a/Å	15.3299(7)
b/Å	17.5645(7)
c/Å	14.9948(9)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4037.5(3)
Z	4
ρ_{calc} g/cm^3	1.373
μ/mm^{-1}	6.322
F(000)	1672.0
Crystal size/mm^3	0.12 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
Theta range for data collection /°	11.804 to 130.116
Index ranges	-18 ≤ h ≤ 17, -20 ≤ k ≤ 20, -17 ≤ l ≤ 17
Reflections collected	21903
Independent reflections	1776 [R_{int} = 0.2266, R_{sigma} = 0.0890]
Data / restraints / parameters	1776/101/149
Goodness-of-fit on F^2	1.183
Final R indexes [I>=2σ (I)]	R_1 = 0.1355, wR_2 = 0.3376
R indices (all data)	R_1 = 0.1374, wR_2 = 0.3380
Largest diff. peak and hole /e Å^{-3}	2.00/-1.24

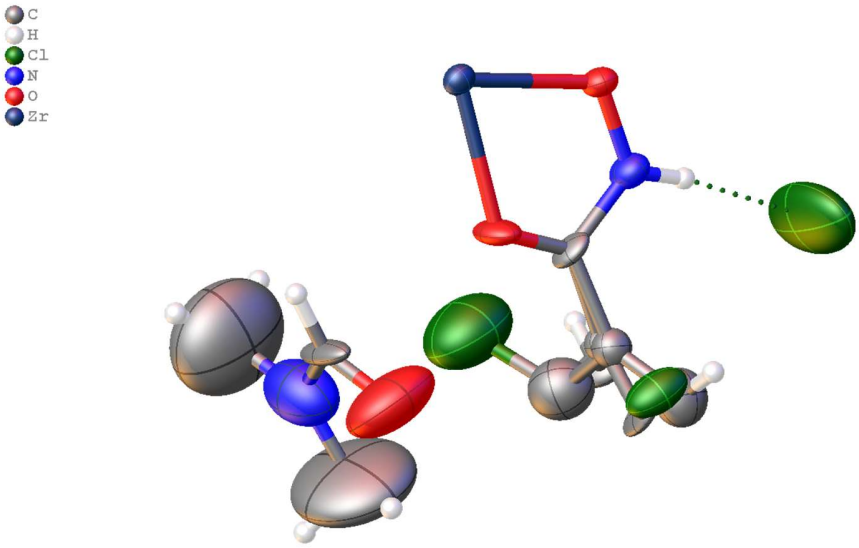

Fig. S13 ORTEP diagram of the asymmetric unit of SUM-1-Cl (50% probability factor for the thermal ellipsoids), generated in Olex2-1.5.

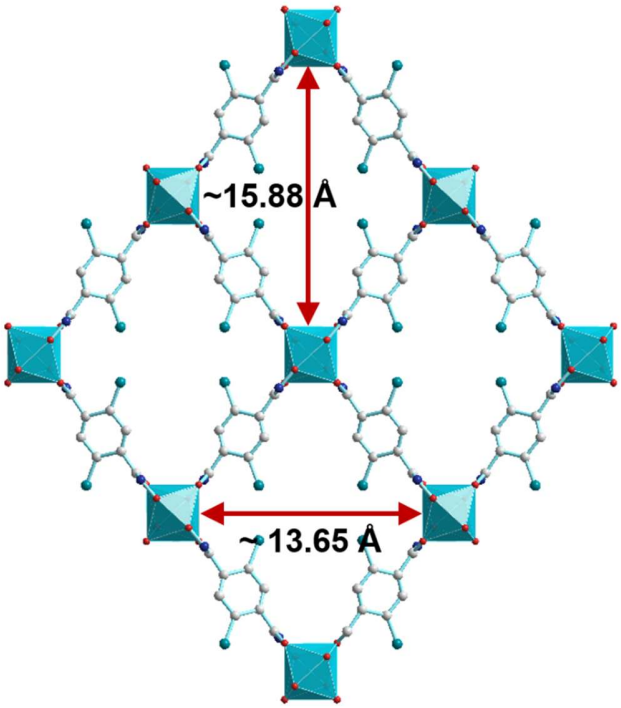

Fig. S14 Crystal structure of SUM-1-Cl, viewed along the *c* axis. Zr: blue polyhedra; C: white spheres; N: dark blue spheres; O: red spheres; F: teal spheres; H: omitted for clarity.

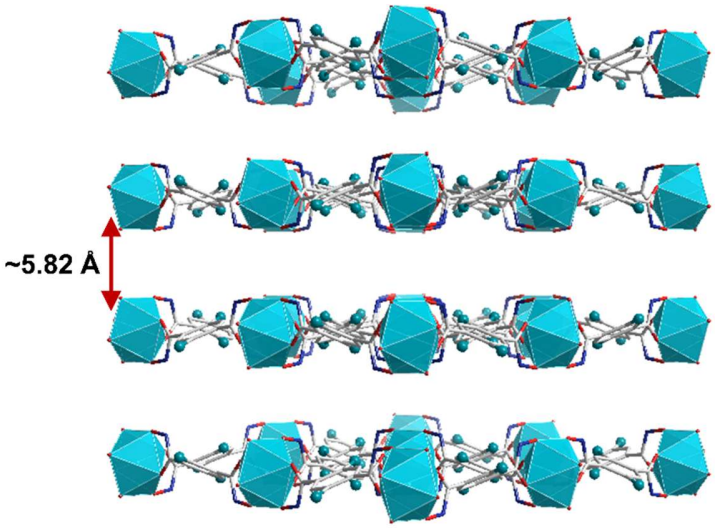

Fig. S15 Crystal structure of SUM-1-Cl, in packed mode, viewed along the *b* axis. Zr: blue polyhedra; C: white spheres; N: dark blue spheres; O: red spheres; F: teal spheres; H: omitted for clarity.

3.3 Crystal structure of SUM-1-Br

Table S3 Crystal data and structure refinement details for SUM-1-Br.

CCDC deposition number	2528073
Compound name	SUM-1-Br
Formula	$C_{32}H_{16}Br_8N_8O_{16}Zr_2$
Formula weight	1590.25
Temperature/K	237.00
Crystal system	tetragonal
Space group	*I4/mcm*
a/Å	16.505(4)
b/Å	16.505(4)
c/Å	15.103(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4114(2)
Z	2
ρ_{calc} g/cm^3	1.284
μ/mm^{-1}	4.180
F(000)	1504.0
Crystal size/mm^3	0.13 × 0.11 × 0.09
Radiation	MoKα (λ = 0.71073)
Theta range for data collection /°	4.936 to 52.75
Index ranges	-20 ≤ h ≤ 20, -20 ≤ k ≤ 20, -18 ≤ l ≤ 17
Reflections collected	23820
Independent reflections	1155 [R_{int} = 0.0620, R_{sigma} = 0.0253]
Data / restraints / parameters	1155/20/61
Goodness-of-fit on F^2	1.145
Final R indexes [I>=2σ (I)]	R_1 = 0.0834, wR_2 = 0.2467
R indices (all data)	R_1 = 0.0904, wR_2 = 0.2536
Largest diff. peak and hole /e Å^{-3}	1.17/-0.76

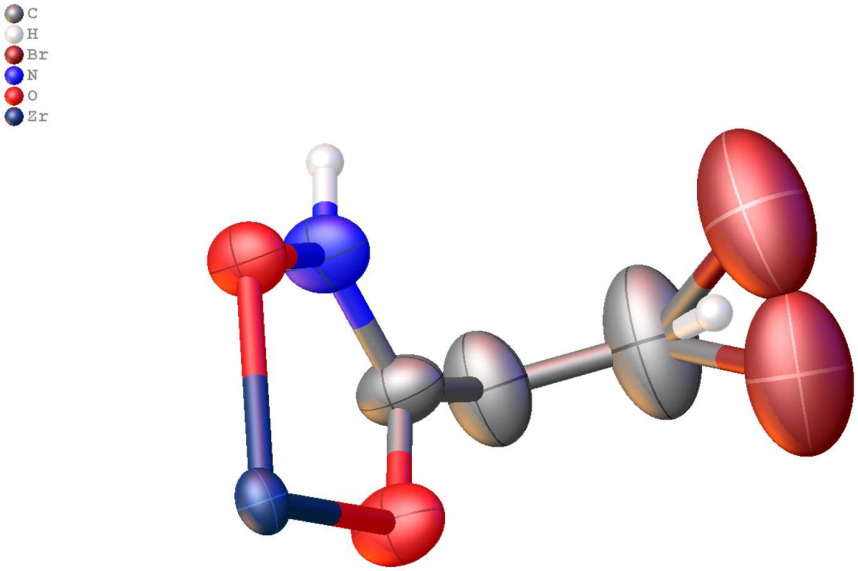

Fig. S16 ORTEP diagram of the asymmetric unit of SUM-1-Br (50% probability factor for the thermal ellipsoids), generated in Olex2-1.5.

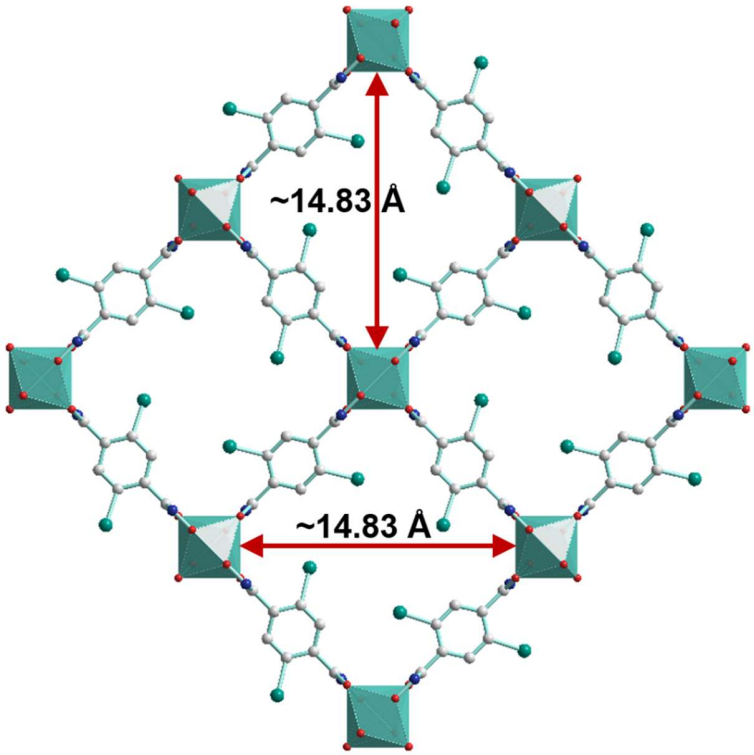

Fig. S17 Crystal structure of SUM-1-Br, viewed along the *c* axis. Zr: green polyhedra; C: white spheres; N: dark blue spheres; O: red spheres; F: teal spheres; H: omitted for clarity.

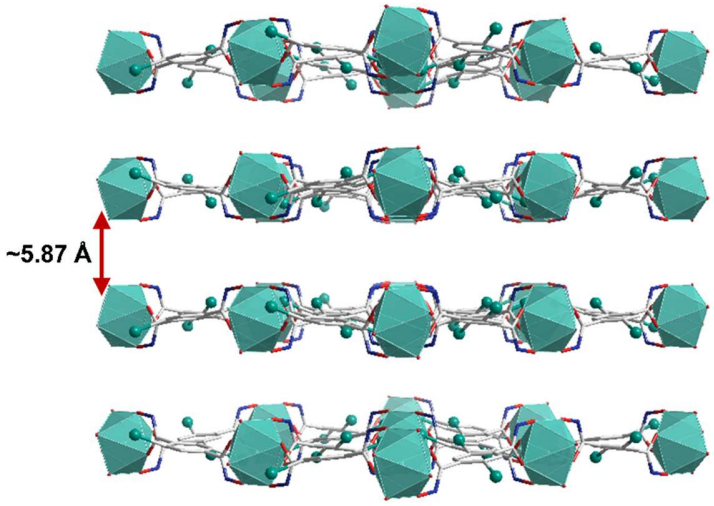

Fig. S18 Crystal structure of SUM-1-Br, in packed mode, viewed along the *b* axis. Zr: green polyhedra; C: white spheres; N: dark blue spheres; O: red spheres; F: teal spheres; H: omitted for clarity.

4. Characterization of SUM-1-F, SUM-1-Cl and SUM-1-Br

4.1 Stability of SUM-1-F, SUM-1-Cl and SUM-1-Br in aqueous solutions with varied pH and organic solvents

For SUM-1-F, SUM-1-Cl and SUM-1-Br, as-synthesized MOFs were washed with dry DMF (3×), then washed (3×) and soaked for 24 hours in aqueous solutions with corresponding pH values. Solutions with different pH were obtained by adding HCl or NaOH to deionized water. After 24 hours, the samples were examined with PXRD.

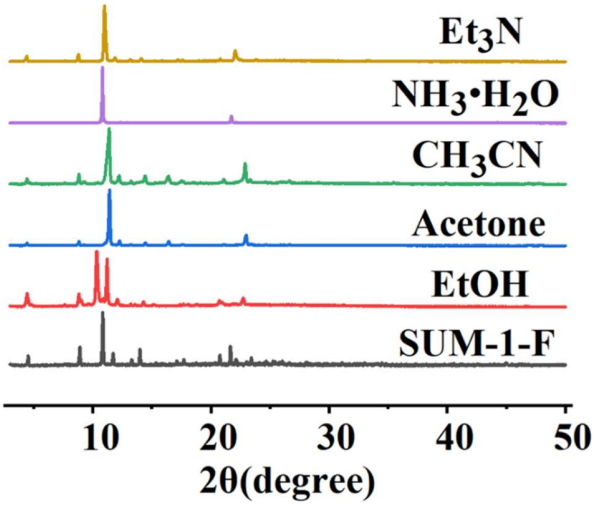

Fig. S19 PXRD patterns of SUM-1-F after soaking in various organic solvents for 24 hours, compared to that of the as-synthesized sample (black).

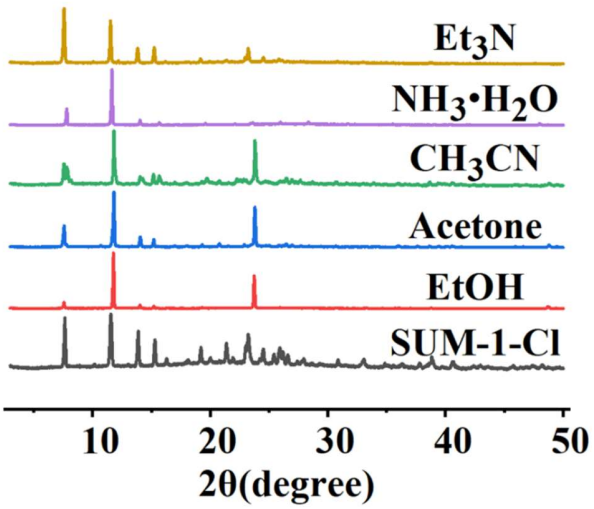

Fig. S20 PXRD patterns of SUM-1-Cl after soaking in various organic solvents for 24 hours, compared to that of the as-synthesized sample (black).

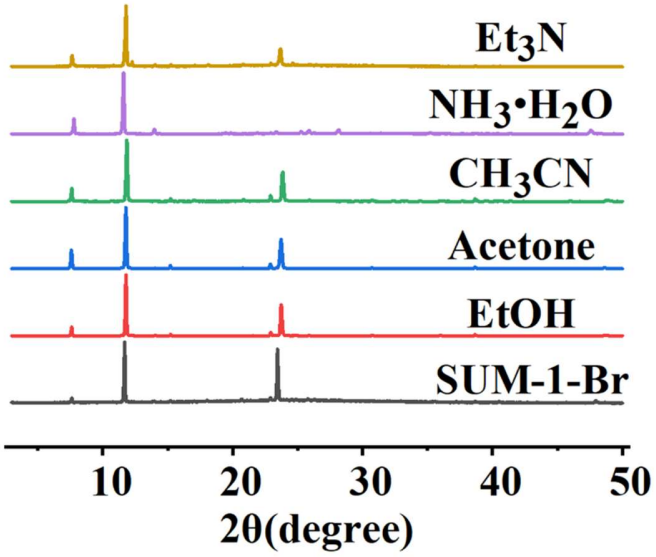

Fig. S21 PXRD patterns of SUM-1-Br after soaking in various organic solvents for 24 hours, compared to that of the as-synthesized sample (black).

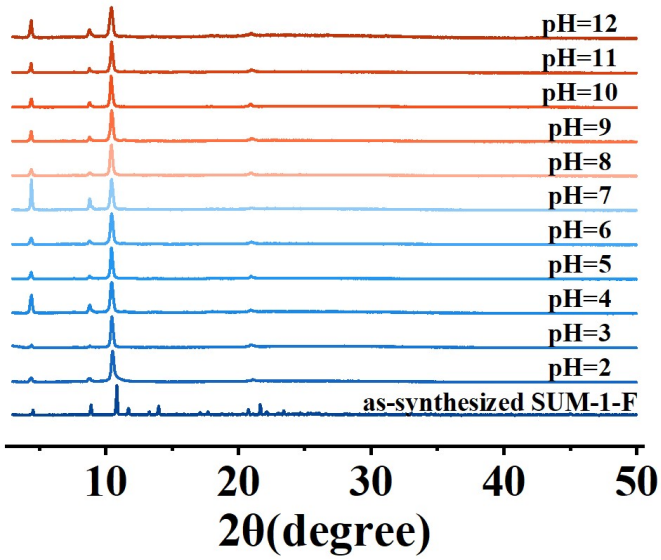

Fig. S22 PXRD patterns of SUM-1-F after soaking in aqueous solutions of indicated pH values for 24 hours, compared to that of the as-synthesized sample (black).

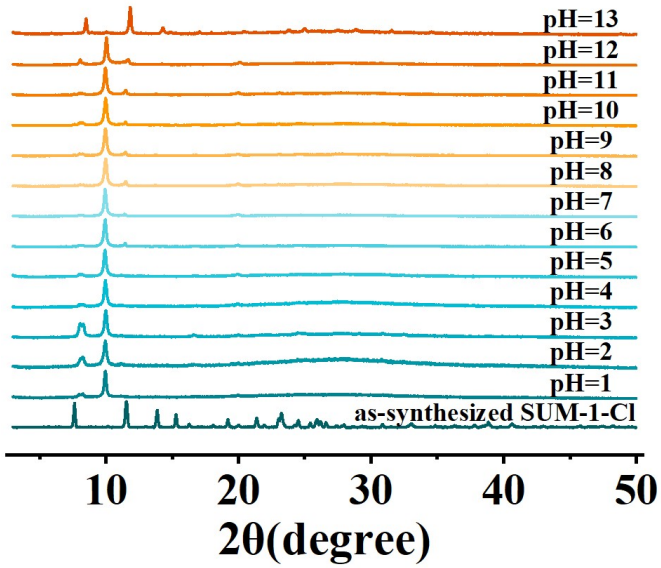

Fig. S23 PXRD patterns of SUM-1-Cl after soaking in aqueous solutions of indicated pH values for 24 hours, compared to that of the as-synthesized sample (black).

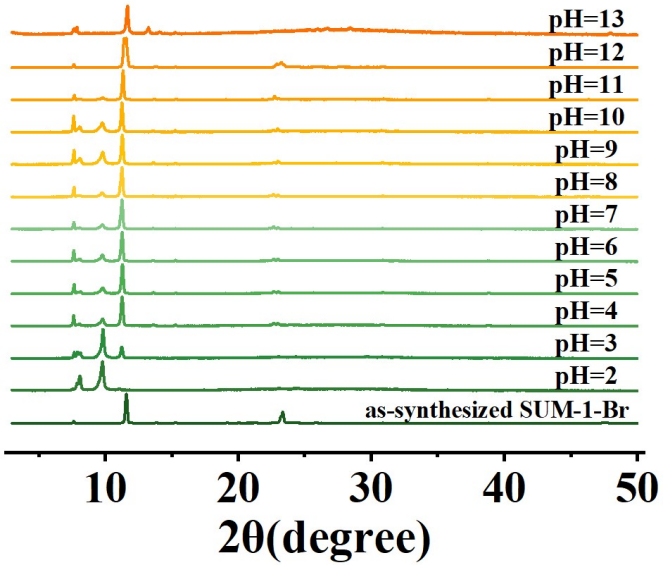

Fig. S24 PXRD patterns of SUM-1-Br after soaking in aqueous solutions of indicated pH values for 24 hours, compared to that of the as-synthesized sample (black).

4.2 Thermogravimetric analysis (TGA) of SUM-1-F, SUM-1-Cl and SUM-1-Br

For TGA, the as-synthesized MOF crystals were washed with dry DMF (3×), dichloromethane (DCM) (3×) and dried with N_2 until they became free-flowing solids, and then loaded into a ceramic pan for analysis.

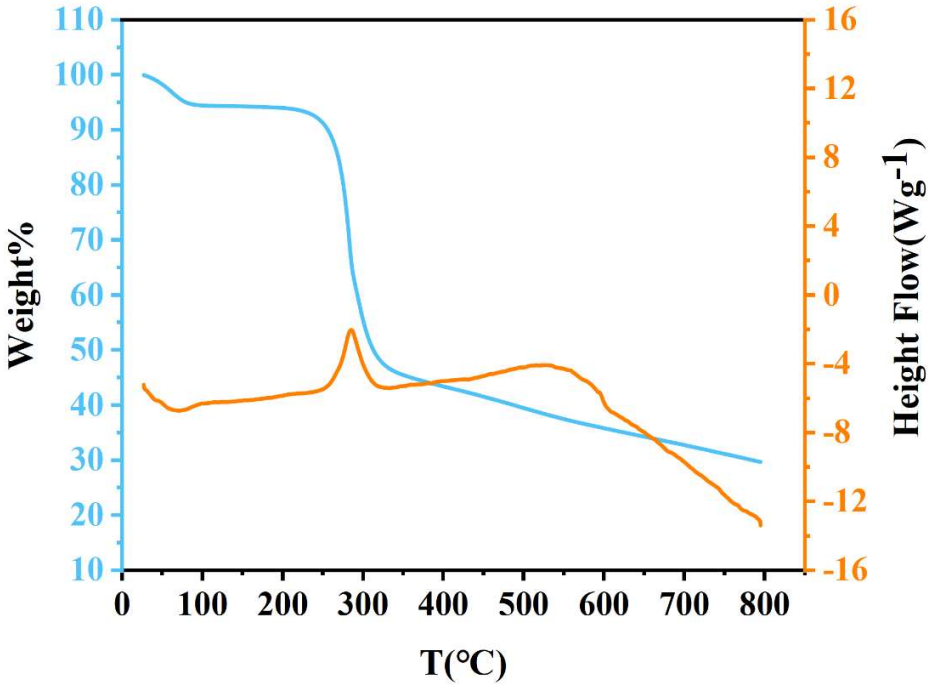

Fig. S25 TGA profile of SUM-1-F.

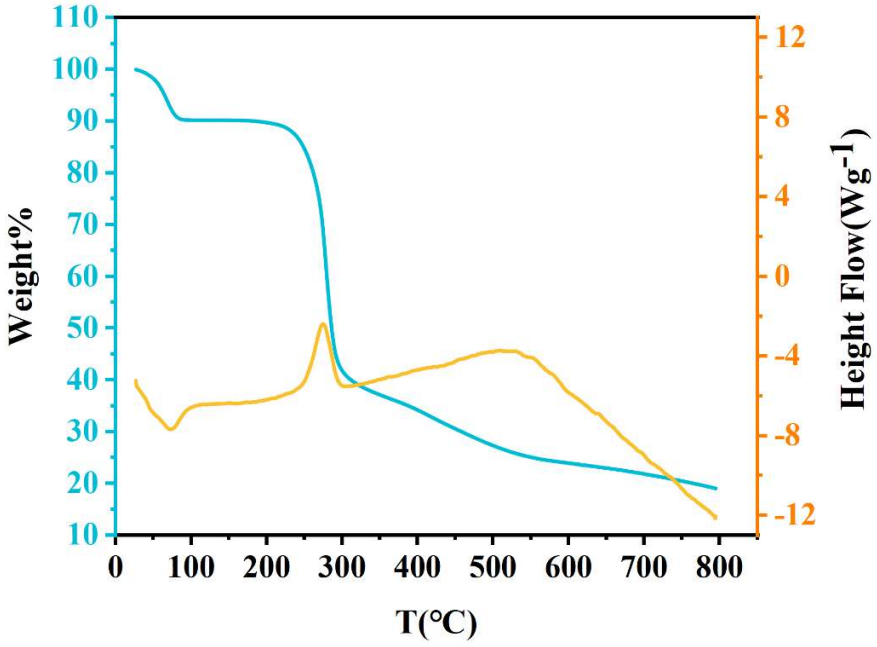

Fig. S26 TGA profile of SUM-1-Cl.

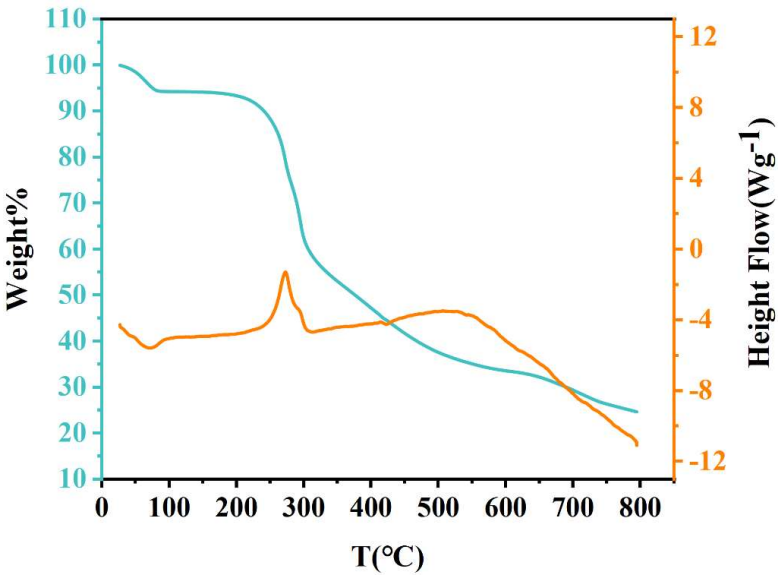

Fig. S27 TGA profile of SUM-1-Br.

4.3 Gas adsorption of SUM-1-F, SUM-1-Cl and SUM-1-Br

The following activation procedure was performed on SUM-1-F, SUM-1-Cl and SUM-1-Br: as-synthesized MOFs were washed with dry DMF (3×) and exchanged with acetone (3×) for 72 h, followed by activation at 100 ºC for 12 h on the degas station of BELSORP MAX. The N_2 adsorption-desorption isotherms were acquired at 77 K.

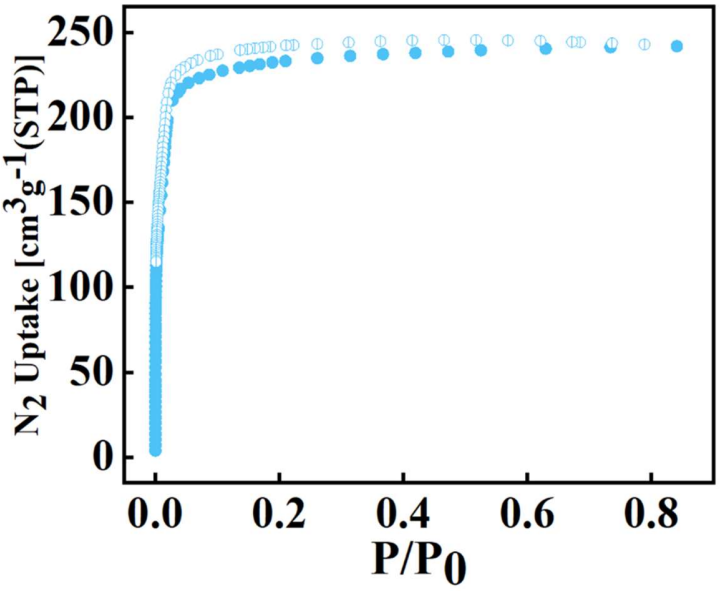

Fig. S28 N_2 adsorption-desorption isotherms of SUM-1-F at 77 K (adsorption: filled circles;

desorption: open circles) .

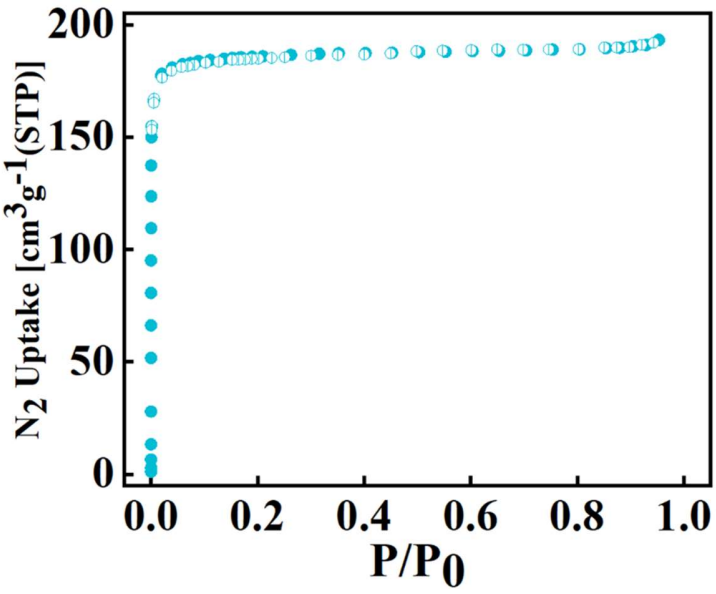

Fig. S29 N_2 adsorption-desorption isotherms of SUM-1-Cl at 77 K (adsorption: filled circles; desorption: open circles) .

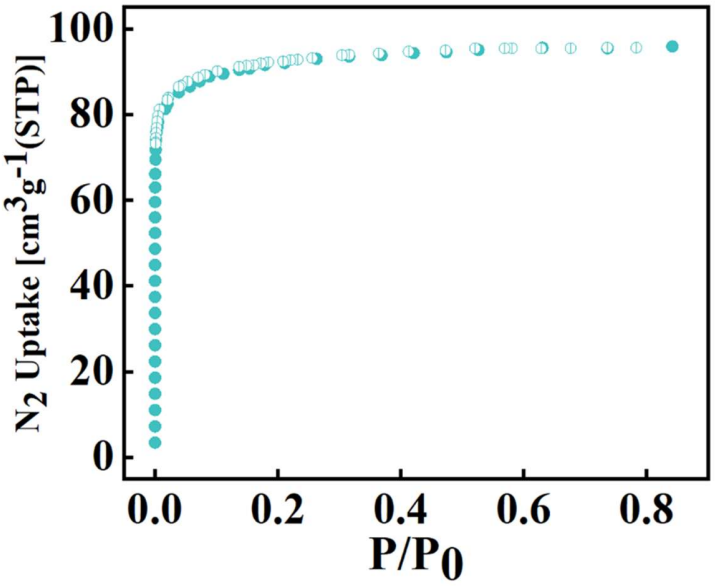

Fig. S30 N_2 adsorption-desorption isotherms of SUM-1-Br at 77 K (adsorption: filled circles; desorption: open circles) .

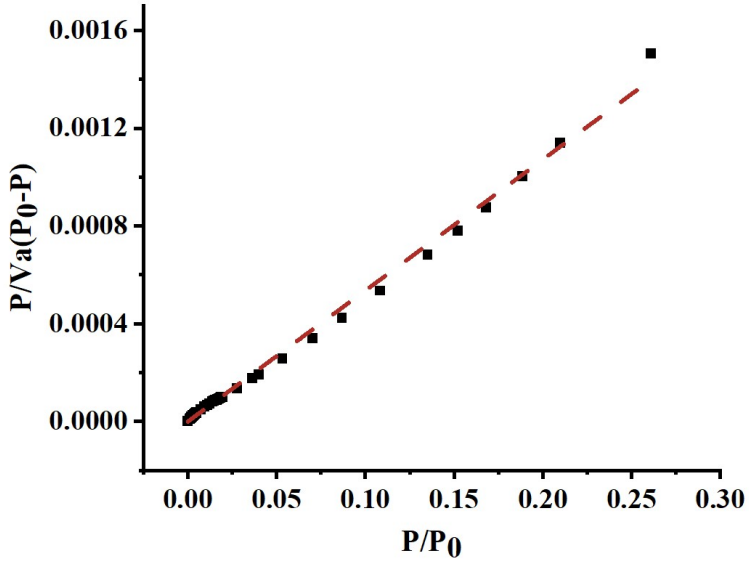

Fig. S31 Specific surface area fitting curve for SUM-1-F.

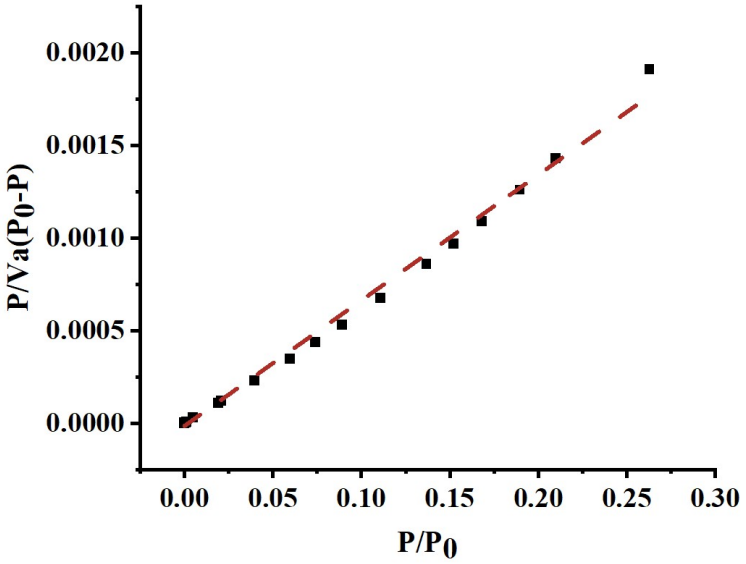

Fig. S32 Specific surface area fitting curve for SUM-1-Cl.

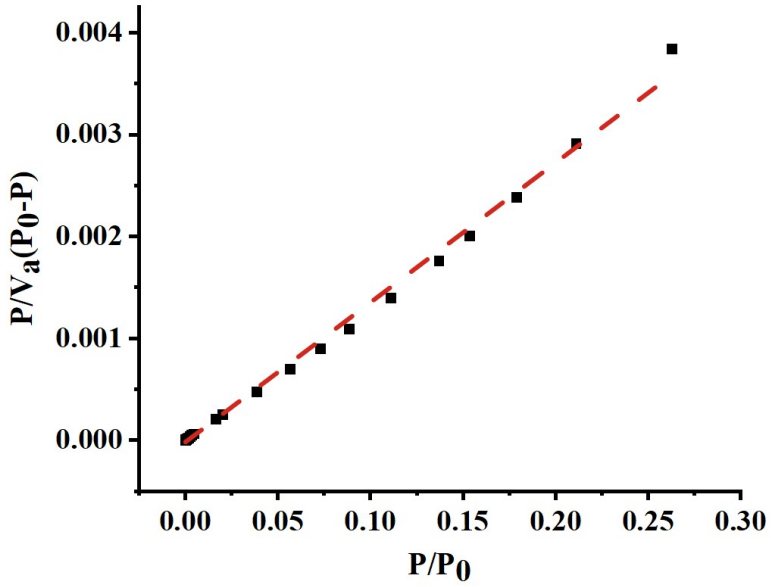

Fig. S33 Specific surface area fitting curve for SUM-1-Br.

5. Synthesis of mono-substituted ligands and attempted synthesis of MOFs

5.1 Synthesis of 2-fluoro-1,4-benzenedihydroxamic acid (H_2-FH-BDHA)[4]

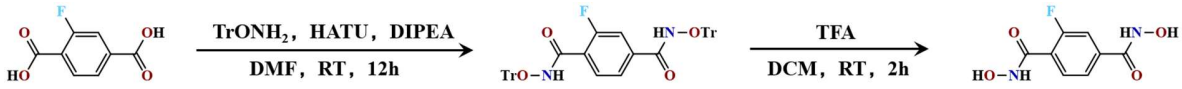

Fig. S34 Synthetic route of H_2-FH-BDHA.

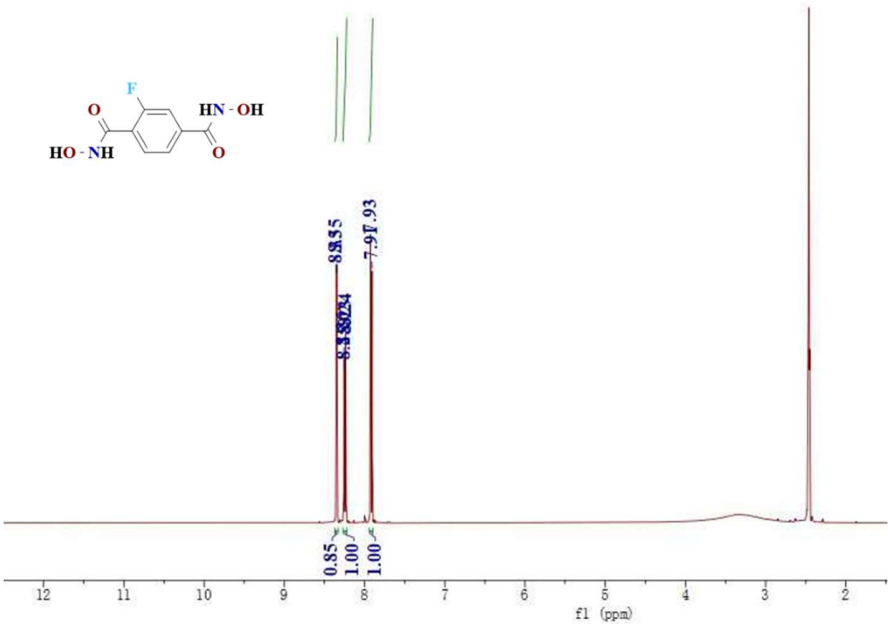

Fig. S35 ^{1}H NMR spectrum of H_2-FH-BDHA in DMSO-d_6.

5.2 Synthesis of 2-chloro-1,4-benzenedihydroxamic acid (H_2-ClH-BDHA)[4]

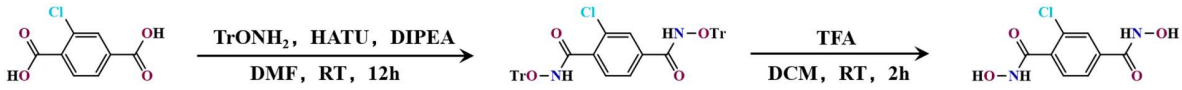

Fig. S36 Synthetic route of H_2-ClH-BDHA.

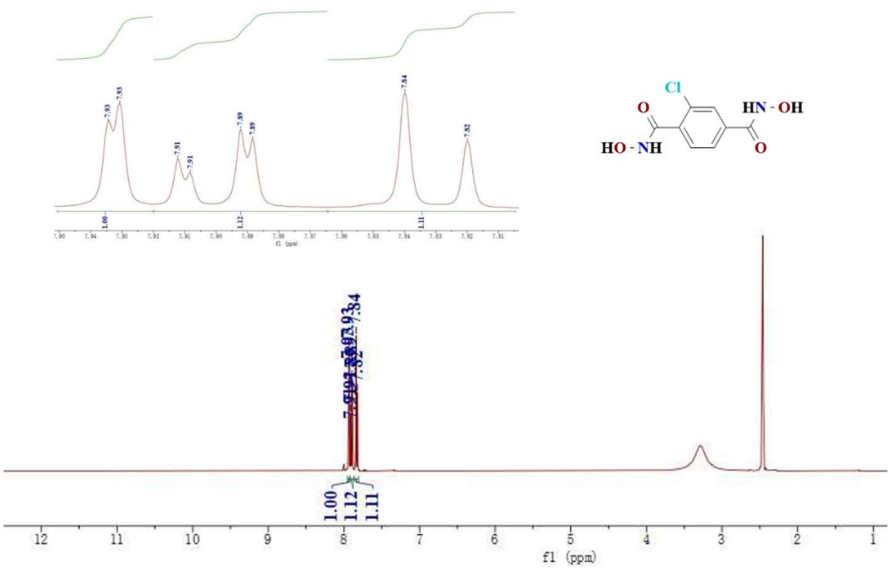

Fig. S37 ^{1}H NMR spectrum of H_2-ClH-BDHA in DMSO-d_6.

5.3 Synthesis of 2-bromo-1,4-benzenedihydroxamic acid (H_2-BrH-BDHA)[4]

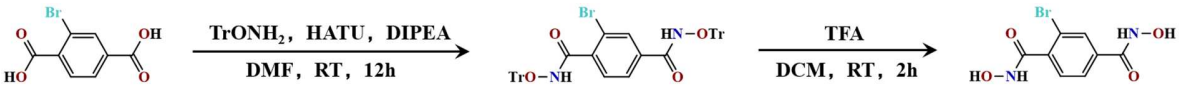

Fig. S38 Synthetic route of H_2-BrH-BDHA.

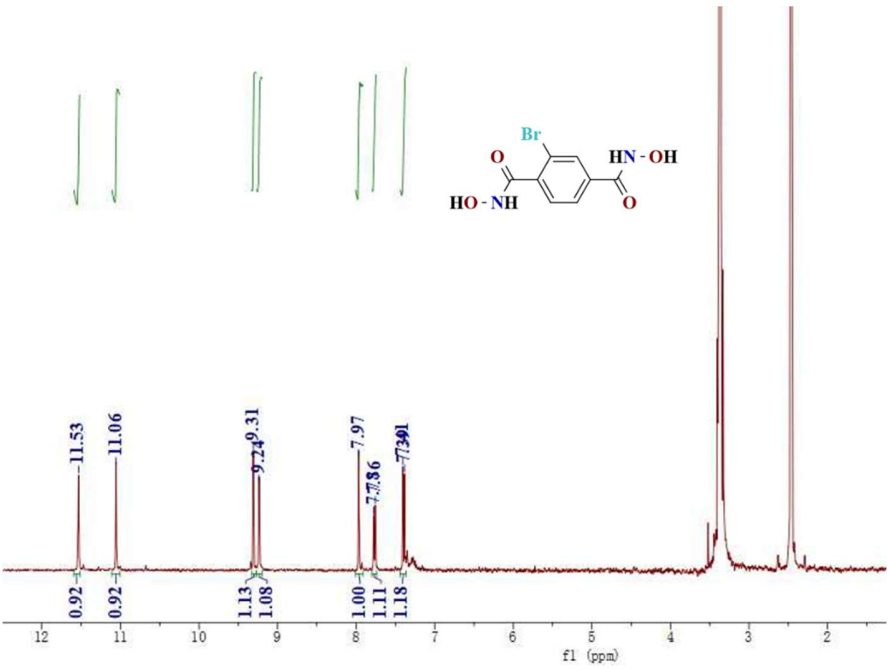

Fig. S39 ^{1}H NMR spectrum of H_2-BrH-BDHA in DMSO-d_6.

5.4 Attempted synthesis of Zr-FH-BDHA MOF

To explore the crystalline assembly of the Zr and H_2-FH-BDHA, a comprehensive screening of synthetic parameters was conducted. Specifically, various acid modulators (e.g. HCl, HNO_3, and H_2SO_4) were introduced to adjust the nucleation rate. Furthermore, wide temperature range (e.g. 50-150°C) and reaction time (e.g. 6h–72h) were tested. Despite these extensive efforts, no crystalline product was obtained; the reaction consistently yielded either clear solutions or amorphous precipitates.

5.5 Attempted synthesis of Zr-ClH-BDHA MOF

To explore the crystalline assembly of the Zr and H_2-ClH-BDHA, a comprehensive screening of synthetic parameters was conducted. Specifically, various acid modulators (e.g. HCl, HNO_3, and H_2SO_4) were introduced to adjust the nucleation rate. Furthermore, wide temperature range (e.g. 50-150°C) and reaction time (e.g. 6h–72h) were tested. Despite these extensive efforts, no crystalline product was obtained; the reaction consistently yielded either clear solutions or amorphous precipitates.

5.6 Attempted synthesis of Zr-BrH-BDHA MOF

To explore the crystalline assembly of the Zr and H_2-BrH-BDHA, a comprehensive screening of synthetic parameters was conducted. Specifically, various acid modulators (e.g. HCl, HNO_3, and H_2SO_4) were introduced to adjust the nucleation rate. Furthermore, wide temperature range (e.g. 50-150°C) and reaction time (e.g. 6h–72h) were tested. Despite these extensive efforts, no crystalline product was obtained; the reaction consistently yielded either clear solutions or amorphous precipitates.

6. Computational method and details

All density functional theory (DFT) calculations in this study were performed using the Gaussian 16[6] software package, and electronic energy calculations for all organic linkers were carried out at the B3LYP level. To achieve a balance between computational efficiency and accuracy, a mixed basis set strategy was employed: the 6-31G basis set was assigned to light atoms (C, H, O, N, and F), while the SDD (Stuttgart-Dresden effective core potential) basis set and its associated pseudopotential were applied to the heavier halogen atoms (Cl and Br). The conformational flexibility of the mono-substituted and di-substituted linkers was investigated via Potential Energy Surface (PES) scans. The scans were performed by incrementally rotating the dihedral angle between the benzene ring and the hydroxamic acid group. For the mono-substituted linkers, the hydroxamic acid group located at the *ortho* position (adjacent to the substituent) and the one at the *meta* position (away from the substituent) were individually rotated (as shown in Fig. S40). In each case, the specified dihedral angle was rotated from 0° to 360° in steps of 30°, sampling a total of 12 conformations. At each step, the specified dihedral angle was constrained while all other internal coordinates were fully optimized, thereby obtaining the energy and electronic properties of the locally optimal structure for each torsional angle. For the di-substituted linkers, the PES scans also considered different rotation modes: one involved the synchronous rotation (in the same or the opposite directions, as shown in Fig. S40) of both hydroxamic acid groups from 0° to 360° in 30° increments; the other involved fixing the dihedral angle of one group while rotating the other group from 0° to 360° in 30° steps. In all scanning steps, only the rotated dihedral angle(s) were allowed to change (or both dihedral angles were allowed to change synchronously in the synchronous rotation mode), while all other internal coordinates were fully optimized to obtain the energy and electronic properties of the optimal structure at each torsional angle.

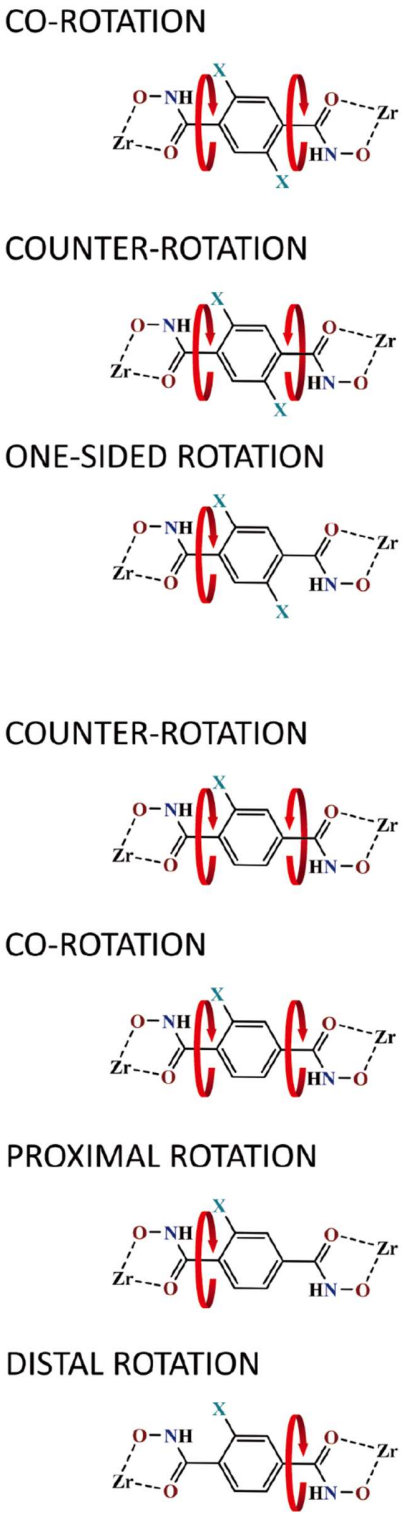

Fig. S40 Illustration of different rotation modes as indicated in Fig. S41, for “di-substituted” (top three) and “mono-substituted” (bottom four) BDHA linkers.

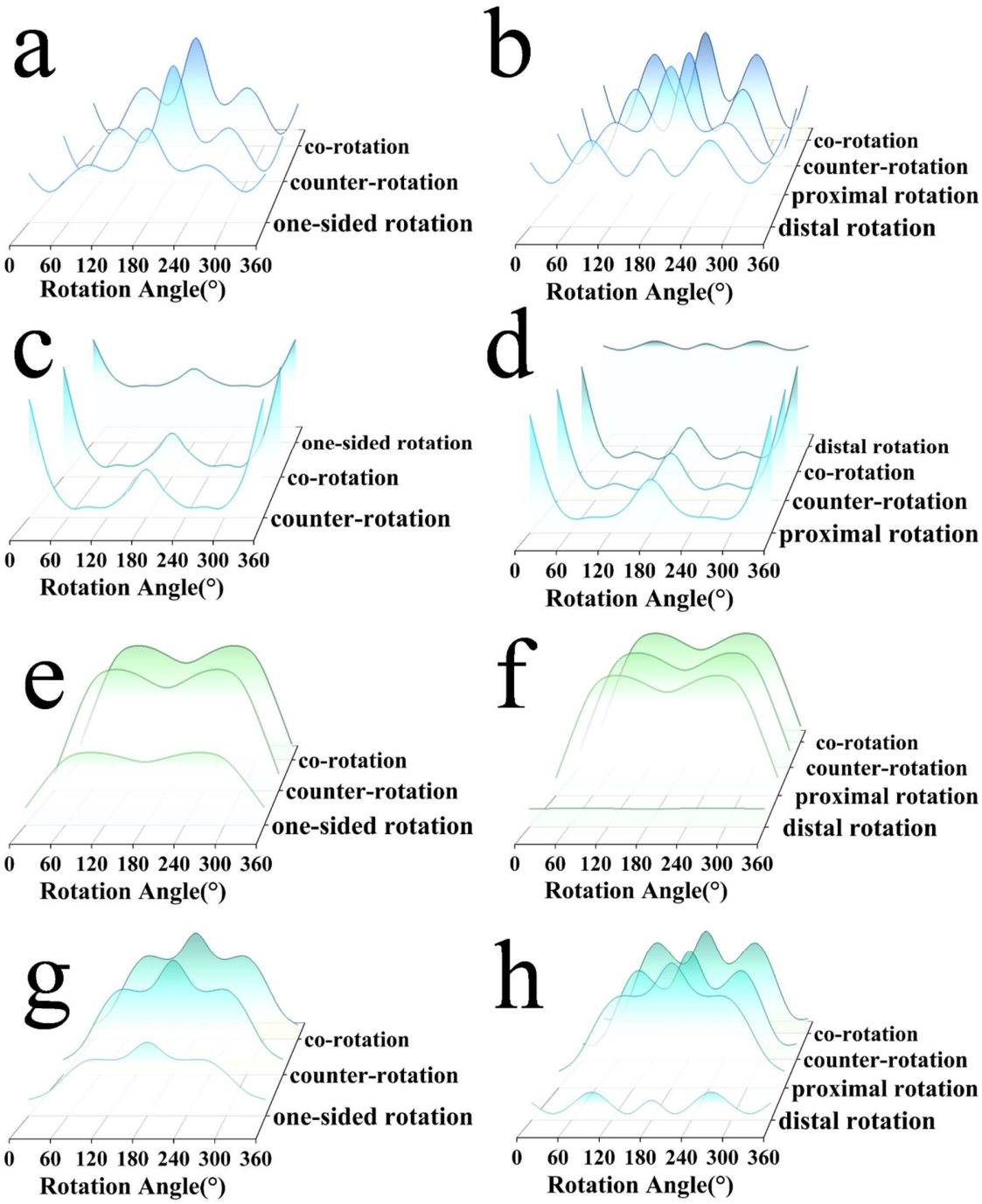

Fig. S41 Conformational energy profiles as a function of dihedral rotation (0–360°) "di-substituted" (a) H_2-F_2-BDHA, (c) H_2-Cl_2-BDHA, (e) H_2-Br_2-BDHA, (g) PZDH linkers, and for "mono-substituted" (b) H_2-FH-BDHA, (d) H_2-ClH-BDHA, (f) H_2-BrH-BDHA and (h) PDDH linkers.

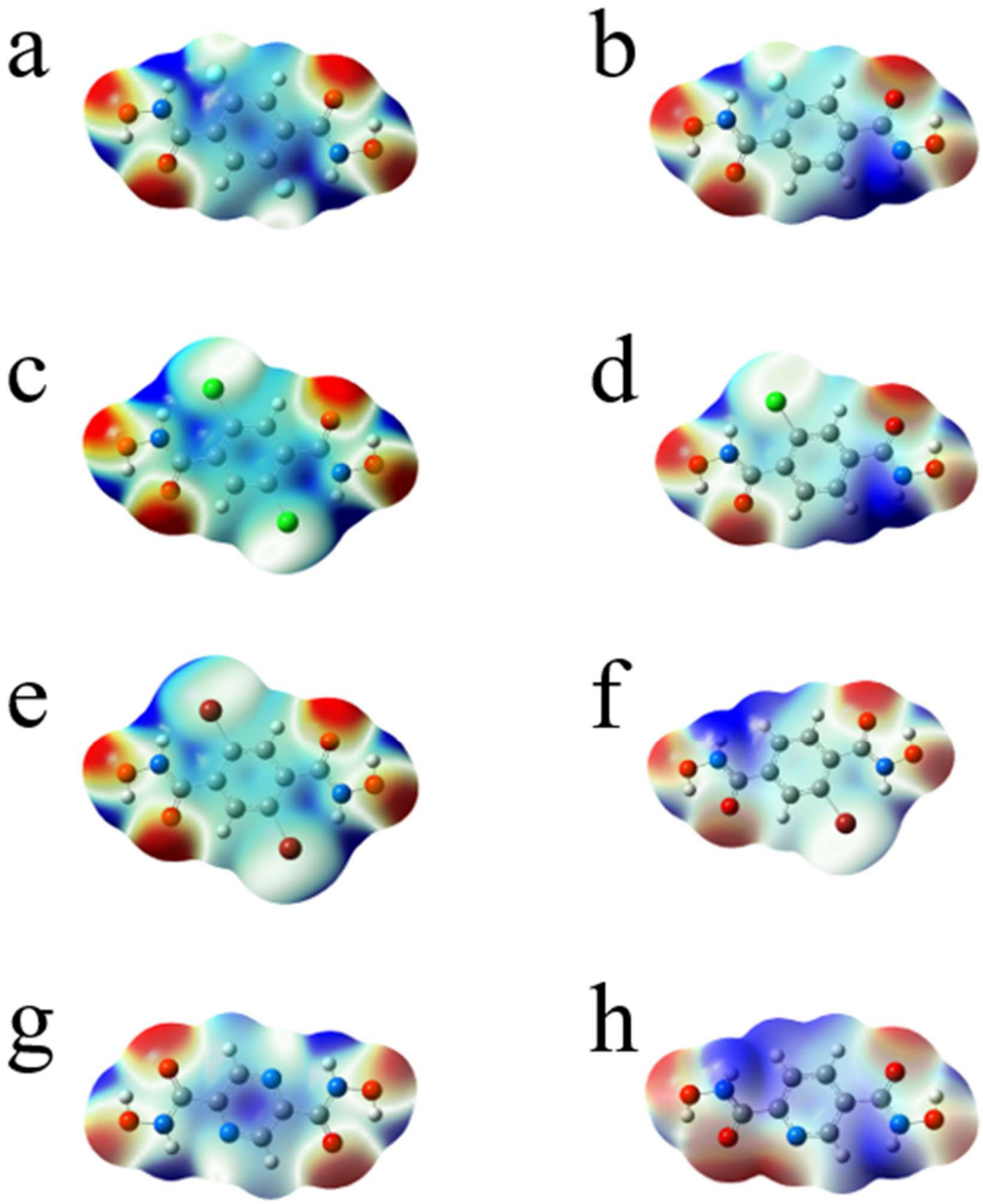

Fig. S42 Electrostatic potential maps for “di-substituted” (a) H_2-F_2-BDHA, (c) H_2-Cl_2-BDHA, (e) H_2-Br_2-BDHA, (g) PZDH linkers, and for “mono-substituted” (b) H_2-FH-BDHA, (d) H_2-ClH-BDHA, (f) H_2-BrH-BDHA and (h) PDDH linkers.

Table S4 Cartesian coordinates of the rotated geometry for the hydroxamate group distal to the F side in the H_2-FH-BDHA ligand.

	0°				30°		
C	0.8484	1.0702	-0.2837	C	0.8484	1.2488	0.1867
C	1.3831	-0.1744	0.0488	C	1.3831	0.0042	0.5192
C	0.5347	-1.2446	0.3326	C	0.5347	-1.066	0.803
C	-0.8483	-1.0701	0.284	C	-0.8483	-0.8915	0.7544
C	-1.383	0.1745	-0.0484	C	-1.383	0.3531	0.422
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.4233	0.1381
C	1.0525	-2.4502	0.6546	C	1.0525	-2.2716	1.125
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.6288	-0.1839
N	-0.2198	3.5006	-0.933	N	-0.3657	3.4676	-1.0199
O	-0.7243	4.6749	-1.2466	O	-0.8702	4.6419	-1.3335
N	0.2198	-3.5005	0.9331	N	0.2198	-3.3219	1.4035
O	0.7243	-4.6749	1.2467	O	0.7243	-4.4963	1.7171
O	-2.2503	2.6014	-0.6964	O	-2.1216	2.9666	0.2658
O	2.2503	-2.6013	0.6967	O	2.2503	-2.4227	1.1671
F	-1.6512	-2.0829	0.5526	F	-1.6512	-1.9043	1.023
H	1.5174	1.9142	-0.5076	H	1.5174	2.0928	-0.0372
H	2.4737	-0.312	0.0872	H	2.4737	-0.1334	0.5576
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.4907	0.3838
H	0.7836	3.374	-0.8977	H	0.5299	3.1847	-1.3966
H	-0.1513	5.3976	-1.4384	H	-0.3976	5.219	-1.9088
H	-0.7836	-3.3739	0.8978	H	-0.7836	-3.1953	1.3682
H	0.1513	-5.3976	1.4384	H	0.1513	-5.219	1.9088
	60°				**90°**		
C	0.8484	1.4789	0.505	C	0.8484	1.6989	0.5858
C	1.3831	0.2343	0.8375	C	1.3831	0.4543	0.9183
C	0.5347	-0.8359	1.1213	C	0.5347	-0.6159	1.2021
C	-0.8483	-0.6614	1.0727	C	-0.8483	-0.4414	1.1535
C	-1.383	0.5832	0.7403	C	-1.383	0.8032	0.8211
C	-0.5346	1.6534	0.4564	C	-0.5346	1.8734	0.5372
C	1.0525	-2.0415	1.4433	C	1.0525	-1.8215	1.5241
C	-1.0525	2.8589	0.1344	C	-1.0525	3.0789	0.2152
N	-0.7659	3.4251	-1.0787	N	-1.3132	3.3844	-1.0937
O	-1.2704	4.5994	-1.3924	O	-1.8177	4.5587	-1.4073
N	0.2198	-3.0918	1.7218	N	0.2198	-2.8718	1.8026
O	0.7243	-4.2662	2.0354	O	0.7243	-4.0462	2.1162
O	-1.7685	3.4373	0.9168	O	-1.2856	3.8874	1.0821
O	2.2503	-2.1926	1.4854	O	2.2503	-1.9726	1.5662
F	-1.6512	-1.6742	1.3413	F	-1.6512	-1.4542	1.4221
H	1.5174	2.3229	0.2811	H	1.5174	2.5429	0.3619
H	2.4737	0.0967	0.8759	H	2.4737	0.3167	0.9567
H	-2.4737	0.7208	0.7021	H	-2.4737	0.9408	0.7829

H	-0.1661	2.9406	-1.7341	H	-1.1179	2.7073	-1.8199
H	-1.0732	4.9889	-2.2271	H	-1.9971	4.7689	-2.3079
H	-0.7836	-2.9652	1.6865	H	-0.7836	-2.7452	1.7673
H	0.1513	-4.9889	2.2271	H	0.1513	-4.7689	2.3079
120°				**150°**			
C	1.0724	1.8499	0.4075	C	1.4113	1.8914	0.0178
C	1.6071	0.6053	0.74	C	1.946	0.6468	0.3503
C	0.7587	-0.4649	1.0238	C	1.0976	-0.4234	0.6341
C	-0.6243	-0.2904	0.9752	C	-0.2854	-0.2489	0.5855
C	-1.159	0.9542	0.6428	C	-0.8201	0.9957	0.2531
C	-0.3106	2.0244	0.3589	C	0.0283	2.0659	-0.0308
C	1.2765	-1.6705	1.3458	C	1.6154	-1.629	0.9561
C	-0.8285	3.2299	0.0369	C	-0.4896	3.2714	-0.3528
N	-1.637	3.3565	-1.0607	N	-1.6996	3.3489	-0.9887
O	-2.1414	4.5308	-1.3744	O	-2.204	4.5231	-1.3024
N	0.4438	-2.7208	1.6243	N	0.7827	-2.6793	1.2346
O	0.9483	-3.8952	1.9379	O	1.2872	-3.8537	1.5482
O	-0.5783	4.1962	0.7174	O	0.1148	4.2811	-0.0796
O	2.4743	-1.8216	1.3879	O	2.8132	-1.7801	0.9982
F	-1.4272	-1.3032	1.2438	F	-1.0883	-1.2617	0.8541
H	1.7414	2.6939	0.1836	H	2.0803	2.7354	-0.2061
H	2.6977	0.4677	0.7784	H	3.0366	0.5092	0.3887
H	-2.2497	1.0918	0.6046	H	-1.9108	1.1333	0.2149
H	-1.8465	2.5471	-1.6308	H	-2.2059	2.5031	-1.2176
H	-2.6977	4.6179	-2.1296	H	-3.0366	4.5764	-1.7399
H	-0.5596	-2.5942	1.589	H	-0.2207	-2.5527	1.1993
H	0.3753	-4.6179	2.1296	H	0.7142	-4.5764	1.7399
180°				**210°**			
C	1.5358	1.8123	-0.4787	C	1.4127	1.6337	-0.3069
C	2.0705	0.5677	-0.1462	C	1.9474	0.3891	0.0256
C	1.2221	-0.5025	0.1376	C	1.099	-0.6811	0.3094
C	-0.1609	-0.328	0.089	C	-0.284	-0.5066	0.2608
C	-0.6956	0.9166	-0.2434	C	-0.8187	0.738	-0.0716
C	0.1528	1.9868	-0.5273	C	0.0297	1.8082	-0.3555
C	1.7399	-1.7081	0.4596	C	1.6168	-1.8867	0.6314
C	-0.3651	3.1923	-0.8493	C	-0.4882	3.0137	-0.6775
N	-1.7226	3.3635	-0.8969	N	-1.6998	3.3965	-0.1677
O	-2.2271	4.5378	-1.2107	O	-2.2043	4.5707	-0.4815
N	0.9072	-2.7584	0.7381	N	0.7841	-2.937	0.9099
O	1.4117	-3.9328	1.0517	O	1.2886	-4.1114	1.2235
O	0.3695	4.1193	-1.0952	O	0.1177	3.7541	-1.4152
O	2.9377	-1.8592	0.5017	O	2.8146	-2.0378	0.6735
F	-0.9638	-1.3408	0.3576	F	-1.0869	-1.5194	0.5294
H	2.2048	2.6563	-0.7026	H	2.0817	2.4777	-0.5308
H	3.1611	0.4301	-0.1078	H	3.038	0.2515	0.064

H	-1.7863	1.0542	-0.2816	H	-1.9094	0.8756	-0.1098
H	-2.338	2.587	-0.691	H	-2.2075	2.7763	0.4502
H	-3.1611	4.6555	-1.2434	H	-3.038	4.8341	-0.1306
H	-0.0962	-2.6318	0.7028	H	-0.2193	-2.8104	0.8746
H	0.8387	-4.6555	1.2434	H	0.7156	-4.8341	1.4152
	240°				**270°**		
C	1.0749	1.4036	-0.1406	C	0.8484	1.1836	-0.0983
C	1.6096	0.159	0.1919	C	1.3831	-0.061	0.2342
C	0.7612	-0.9112	0.4757	C	0.5347	-1.1312	0.518
C	-0.6218	-0.7367	0.4271	C	-0.8483	-0.9567	0.4694
C	-1.1565	0.5079	0.0947	C	-1.383	0.2879	0.137
C	-0.3081	1.5781	-0.1892	C	-0.5346	1.3581	-0.1469
C	1.279	-2.1168	0.7977	C	1.0525	-2.3368	0.84
C	-0.826	2.7836	-0.5112	C	-1.0525	2.5636	-0.4689
N	-1.6374	3.439	0.3757	N	-1.3166	3.4797	0.5136
O	-2.1419	4.6133	0.062	O	-1.8211	4.6539	0.2
N	0.4463	-3.1671	1.0762	N	0.2198	-3.3871	1.1185
O	0.9508	-4.3415	1.3898	O	0.7243	-4.5615	1.4321
O	-0.5732	3.2834	-1.5815	O	-1.2826	2.8333	-1.6238
O	2.4768	-2.2679	0.8398	O	2.2503	-2.4879	0.8821
F	-1.4247	-1.7495	0.6957	F	-1.6512	-1.9695	0.738
H	1.7439	2.2476	-0.3645	H	1.5174	2.0276	-0.3222
H	2.7002	0.0214	0.2303	H	2.4737	-0.1986	0.2726
H	-2.2472	0.6455	0.0565	H	-2.4737	0.4255	0.0988
H	-1.8493	3.0204	1.2723	H	-1.1239	3.2537	1.4811
H	-2.7002	5.0642	0.6722	H	-2.0028	5.2842	0.8761
H	-0.5571	-3.0405	1.0409	H	-0.7836	-3.2605	1.0832
H	0.3778	-5.0642	1.5815	H	0.1513	-5.2842	1.6238
	300°				**330°**		
C	0.8484	1.0326	-0.1915	C	0.8484	0.9911	-0.3952
C	1.3831	-0.212	0.141	C	1.3831	-0.2535	-0.0627
C	0.5347	-1.2822	0.4248	C	0.5347	-1.3237	0.2211
C	-0.8483	-1.1077	0.3762	C	-0.8483	-1.1492	0.1725
C	-1.383	0.1369	0.0438	C	-1.383	0.0954	-0.1599
C	-0.5346	1.2071	-0.2401	C	-0.5346	1.1656	-0.4438
C	1.0525	-2.4878	0.7468	C	1.0525	-2.5293	0.5431
C	-1.0525	2.4126	-0.5621	C	-1.0525	2.3711	-0.7658
N	-0.7688	3.5076	0.2092	N	-0.3674	3.5152	-0.4561
O	-1.2733	4.6818	-0.1045	O	-0.8719	4.6895	-0.7697
N	0.2198	-3.5381	1.0253	N	0.2198	-3.5796	0.8216
O	0.7243	-4.7125	1.3389	O	0.7243	-4.754	1.1352
O	-1.7659	2.5244	-1.5306	O	-2.1201	2.4396	-1.3269
O	2.2503	-2.6389	0.7889	O	2.2503	-2.6804	0.5852
F	-1.6512	-2.1205	0.6448	F	-1.6512	-2.162	0.4411
H	1.5174	1.8766	-0.4154	H	1.5174	1.8351	-0.6191

H	2.4737	-0.3496	0.1794	H	2.4737	-0.3911	-0.0243
H	-2.4737	0.2745	0.0056	H	-2.4737	0.233	-0.1981
H	-0.1712	3.4139	1.0205	H	0.5269	3.4579	0.014
H	-1.0781	5.4352	0.4262	H	-0.4004	5.4767	-0.5567
H	-0.7836	-3.4115	0.99	H	-0.7836	-3.453	0.7863
H	0.1513	-5.4352	1.5306	H	0.1513	-5.4767	1.3269

Table S5 Cartesian coordinates of the rotated geometry for the hydroxamate group proximal to the F side in the H_2-FH-BDHA ligand.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.935	1.191	-0.132
C	1.3831	-0.1744	0.0488	C	1.136	0.037	0.626
C	0.5347	-1.2446	0.3326	C	0.2	-0.997	0.582
C	-0.8483	-1.0701	0.284	C	-0.935	-0.877	-0.219
C	-1.383	0.1745	-0.0484	C	-1.136	0.278	-0.976
C	-0.5346	1.2447	-0.3323	C	-0.2	1.311	-0.932
C	1.0525	-2.4502	0.6546	C	0.394	-2.115	1.315
C	-1.0525	2.4502	-0.6543	C	-0.394	2.429	-1.666
N	-0.2198	3.5006	-0.933	N	0.524	3.444	-1.623
O	-0.7243	4.6749	-1.2466	O	0.335	4.533	-2.338
N	0.2198	-3.5005	0.9331	N	-0.094	-3.316	0.875
O	0.7243	-4.6749	1.2467	O	0.095	-4.404	1.59
O	-2.2503	2.6014	-0.6964	O	-1.378	2.533	-2.359
O	2.2503	-2.6013	0.6967	O	0.999	-2.055	2.359
F	-1.6512	-2.0829	0.5526	F	-1.82	-1.855	-0.26
H	1.5174	1.9142	-0.5076	H	1.673	2.006	-0.097
H	2.4737	-0.312	0.0872	H	2.031	-0.058	1.257
H	-2.4737	0.3121	-0.0866	H	-2.031	0.372	-1.608
H	0.7836	3.374	-0.8977	H	1.348	3.357	-1.042
H	-0.1513	5.3976	-1.4384	H	0.967	5.231	-2.308
H	-0.7836	-3.3739	0.8978	H	-0.601	-3.366	0.001
H	0.1513	-5.3976	1.4384	H	-0.242	-5.231	1.287
60°				**90°**			
C	0.935	1.2045	-0.2115	C	0.935	1.071	-0.1735
C	1.136	0.0505	0.5465	C	1.136	-0.083	0.5845
C	0.2	-0.9835	0.5025	C	0.2	-1.117	0.5405
C	-0.935	-0.8635	-0.2985	C	-0.935	-0.997	-0.2605
C	-1.136	0.2915	-1.0555	C	-1.136	0.158	-1.0175
C	-0.2	1.3245	-1.0115	C	-0.2	1.191	-0.9735
C	0.394	-2.1015	1.2355	C	0.394	-2.235	1.2735
C	-0.394	2.4425	-1.7455	C	-0.394	2.309	-1.7075
N	0.524	3.4575	-1.7025	N	0.524	3.324	-1.6645
O	0.335	4.5465	-2.4175	O	0.335	4.413	-2.3795
N	0.492	-3.3185	0.6165	N	1.079	-3.293	0.7405

O	0.681	-4.4075	1.3305	O	1.268	-4.382	1.4545
O	-1.378	2.5465	-2.4385	O	-1.378	2.413	-2.4005
O	0.481	-2.0275	2.4385	O	-0.036	-2.3	2.4005
F	-1.82	-1.8415	-0.3395	F	-1.82	-1.975	-0.3015
H	1.673	2.0195	-0.1765	H	1.673	1.886	-0.1385
H	2.031	-0.0445	1.1775	H	2.031	-0.178	1.2155
H	-2.031	0.3855	-1.6875	H	-2.031	0.252	-1.6495
H	1.348	3.3705	-1.1215	H	1.348	3.237	-1.0835
H	0.967	5.2445	-2.3875	H	0.967	5.111	-2.3495
H	0.419	-3.3805	-0.3915	H	1.44	-3.239	-0.2035
H	0.748	-5.2445	0.9045	H	1.739	-5.111	1.0875
	120°				**150°**		
C	0.7185	0.826	-0.0285	C	0.5855	0.5355	-0.202
C	0.9195	-0.328	0.7295	C	0.7865	-0.6185	0.556
C	-0.0165	-1.362	0.6855	C	-0.1495	-1.6525	0.512
C	-1.1515	-1.242	-0.1155	C	-1.2845	-1.5325	-0.289
C	-1.3525	-0.087	-0.8725	C	-1.4855	-0.3775	-1.046
C	-0.4165	0.946	-0.8285	C	-0.5495	0.6555	-1.002
C	0.1775	-2.48	1.4185	C	0.0445	-2.7705	1.245
C	-0.6105	2.064	-1.5625	C	-0.7435	1.7735	-1.736
N	0.3075	3.079	-1.5195	N	0.1745	2.7885	-1.693
O	0.1185	4.168	-2.2345	O	-0.0145	3.8775	-2.408
N	1.2925	-3.248	1.2135	N	1.3165	-3.1945	1.523
O	1.4815	-4.337	1.9285	O	1.5055	-4.2835	2.238
O	-1.5945	2.168	-2.2555	O	-1.7275	1.8775	-2.429
O	-0.6315	-2.801	2.2555	O	-0.9035	-3.3955	1.656
F	-2.0365	-2.22	-0.1565	F	-2.1695	-2.5105	-0.33
H	1.4565	1.641	0.0065	H	1.3235	1.3505	-0.167
H	1.8145	-0.423	1.3605	H	1.6815	-0.7135	1.187
H	-2.2475	0.007	-1.5045	H	-2.3805	-0.2835	-1.678
H	1.1315	2.992	-0.9385	H	0.9985	2.7015	-1.112
H	0.7505	4.866	-2.2045	H	0.6175	4.5755	-2.378
H	1.9705	-2.979	0.5125	H	2.1115	-2.6705	1.179
H	2.2475	-4.866	1.7865	H	2.3805	-4.5755	2.429
	180°				**210°**		
C	0.718	0.277	-0.631	C	0.935	0.1625	-0.966
C	0.919	-0.877	0.127	C	1.136	-0.9915	-0.208
C	-0.017	-1.911	0.083	C	0.2	-2.0255	-0.252
C	-1.152	-1.791	-0.718	C	-0.935	-1.9055	-1.053
C	-1.353	-0.636	-1.475	C	-1.136	-0.7505	-1.81
C	-0.417	0.397	-1.431	C	-0.2	0.2825	-1.766
C	0.177	-3.029	0.816	C	0.394	-3.1435	0.481
C	-0.611	1.515	-2.165	C	-0.394	1.4005	-2.5
N	0.307	2.53	-2.122	N	0.524	2.4155	-2.457
O	0.118	3.619	-2.837	O	0.335	3.5045	-3.172

N	1.292	-3.147	1.602	N	1.08	-3.0755	1.665
O	1.481	-4.236	2.317	O	1.269	-4.1645	2.379
O	-1.595	1.619	-2.858	O	-1.378	1.5045	-3.193
O	-0.633	-3.924	0.779	O	-0.037	-4.2025	0.093
F	-2.037	-2.769	-0.759	F	-1.82	-2.8835	-1.094
H	1.456	1.092	-0.596	H	1.673	0.9775	-0.931
H	1.814	-0.972	0.758	H	2.031	-1.0865	0.423
H	-2.248	-0.542	-2.107	H	-2.031	-0.6565	-2.442
H	1.131	2.443	-1.541	H	1.348	2.3285	-1.876
H	0.75	4.317	-2.807	H	0.967	4.2025	-3.142
H	1.971	-2.397	1.634	H	1.441	-2.1875	1.99
H	2.248	-4.317	2.858	H	1.74	-4.1175	3.193
	240°				**270°**		
C	0.935	0.17	-1.1175	C	0.935	0.24	-1.045
C	1.136	-0.984	-0.3595	C	1.136	-0.914	-0.287
C	0.2	-2.018	-0.4035	C	0.2	-1.948	-0.331
C	-0.935	-1.898	-1.2045	C	-0.935	-1.828	-1.132
C	-1.136	-0.743	-1.9615	C	-1.136	-0.673	-1.889
C	-0.2	0.29	-1.9175	C	-0.2	0.36	-1.845
C	0.394	-3.136	0.3295	C	0.394	-3.066	0.402
C	-0.394	1.408	-2.6515	C	-0.394	1.478	-2.579
N	0.524	2.423	-2.6085	N	0.524	2.493	-2.536
O	0.335	3.512	-3.3235	O	0.335	3.582	-3.251
N	0.493	-3.052	1.6925	N	-0.094	-3.14	1.679
O	0.682	-4.141	2.4075	O	0.095	-4.229	2.394
O	-1.378	1.512	-3.3445	O	-1.378	1.582	-3.272
O	0.481	-4.21	-0.2165	O	0.998	-4	-0.069
F	-1.82	-2.876	-1.2455	F	-1.82	-2.806	-1.173
H	1.673	0.985	-1.0825	H	1.673	1.055	-1.01
H	2.031	-1.079	0.2715	H	2.031	-1.009	0.344
H	-2.031	-0.649	-2.5935	H	-2.031	-0.579	-2.521
H	1.348	2.336	-2.0275	H	1.348	2.406	-1.955
H	0.967	4.21	-3.2935	H	0.967	4.28	-3.221
H	0.421	-2.152	2.1505	H	-0.6	-2.357	2.074
H	0.75	-4.083	3.3445	H	-0.24	-4.28	3.272
	300°				**330°**		
C	0.935	0.485	-0.768	C	0.935	0.7755	-0.36
C	1.136	-0.669	-0.01	C	1.136	-0.3785	0.398
C	0.2	-1.703	-0.054	C	0.2	-1.4125	0.354
C	-0.935	-1.583	-0.855	C	-0.935	-1.2925	-0.447
C	-1.136	-0.428	-1.612	C	-1.136	-0.1375	-1.204
C	-0.2	0.605	-1.568	C	-0.2	0.8955	-1.16
C	0.394	-2.821	0.679	C	0.394	-2.5305	1.087
C	-0.394	1.723	-2.302	C	-0.394	2.0135	-1.894
N	0.524	2.738	-2.259	N	0.524	3.0285	-1.851

O	0.335	3.827	-2.974	O	0.335	4.1175	-2.566
N	-0.523	-3.185	1.628	N	-0.681	-3.2385	1.553
O	-0.334	-4.274	2.342	O	-0.492	-4.3275	2.267
O	-1.378	1.827	-2.995	O	-1.378	2.1175	-2.587
O	1.378	-3.499	0.498	O	1.516	-2.9045	1.333
F	-1.82	-2.561	-0.896	F	-1.82	-2.2705	-0.488
H	1.673	1.3	-0.733	H	1.673	1.5905	-0.325
H	2.031	-0.764	0.621	H	2.031	-0.4735	1.029
H	-2.031	-0.334	-2.244	H	-2.031	-0.0435	-1.836
H	1.348	2.651	-1.678	H	1.348	2.9415	-1.27
H	0.967	4.525	-2.944	H	0.967	4.8155	-2.536
H	-1.347	-2.617	1.78	H	-1.621	-2.9255	1.347
H	-0.966	-4.525	2.995	H	-1.231	-4.8155	2.587

Table S6 Cartesian coordinates of the H_2-FH-BDHA ligand geometry after co-rotation of both hydroxamate groups.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.8484	1.0702	-0.2839
C	1.3831	-0.1744	0.0488	C	1.3831	-0.1744	0.0486
C	0.5347	-1.2446	0.3326	C	0.5347	-1.2446	0.3324
C	-0.8483	-1.0701	0.284	C	-0.8483	-1.0701	0.2838
C	-1.383	0.1745	-0.0484	C	-1.383	0.1745	-0.0486
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.2447	-0.3325
C	1.0525	-2.4502	0.6546	C	1.0525	-2.4502	0.6544
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.4502	-0.6545
N	-0.2198	3.5006	-0.933	N	-0.3674	3.5943	-0.3448
O	-0.7243	4.6749	-1.2466	O	-0.8719	4.7686	-0.6584
N	0.2198	-3.5005	0.9331	N	0.3674	-3.5943	0.3447
O	0.7243	-4.6749	1.2467	O	0.8719	-4.7686	0.6583
O	-2.2503	2.6014	-0.6964	O	-2.1201	2.5187	-1.2157
O	2.2503	-2.6013	0.6967	O	2.1201	-2.5186	1.2157
F	-1.6512	-2.0829	0.5526	F	-1.6512	-2.0829	0.5524
H	1.5174	1.9142	-0.5076	H	1.5174	1.9142	-0.5078
H	2.4737	-0.312	0.0872	H	2.4737	-0.312	0.087
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.3121	-0.0868
H	0.7836	3.374	-0.8977	H	0.5269	3.537	0.1253
H	-0.1513	5.3976	-1.4384	H	-0.4004	5.5558	-0.4454
H	-0.7836	-3.3739	0.8978	H	-0.5269	-3.5369	-0.1255
H	0.1513	-5.3976	1.4384	H	0.4005	-5.5558	0.4452
60°				**90°**			
C	0.8484	1.0702	-0.2839	C	0.8484	1.0702	-0.2839
C	1.3831	-0.1744	0.0486	C	1.3831	-0.1744	0.0486
C	0.5347	-1.2446	0.3324	C	0.5347	-1.2446	0.3324
C	-0.8483	-1.0701	0.2838	C	-0.8483	-1.0701	0.2838

C	-1.383	0.1745	-0.0486	C	-1.383	0.1745	-0.0486
C	-0.5346	1.2447	-0.3325	C	-0.5346	1.2447	-0.3325
C	1.0525	-2.4502	0.6544	C	1.0525	-2.4502	0.6544
C	-1.0525	2.4502	-0.6545	C	-1.0525	2.4502	-0.6545
N	-0.7688	3.5452	0.1168	N	-1.3166	3.3663	0.3281
O	-1.2733	4.7194	-0.1968	O	-1.8211	4.5406	0.0144
N	0.7689	-3.5451	-0.1169	N	1.3166	-3.3662	-0.328
O	1.2734	-4.7195	0.1968	O	1.8211	-4.5406	-0.0143
O	-1.7659	2.562	-1.623	O	-1.2826	2.7199	-1.8093
O	1.7658	-2.562	1.623	O	1.2824	-2.7198	1.8093
F	-1.6512	-2.0829	0.5524	F	-1.6512	-2.0829	0.5524
H	1.5174	1.9142	-0.5078	H	1.5174	1.9142	-0.5078
H	2.4737	-0.312	0.087	H	2.4737	-0.312	0.087
H	-2.4737	0.3121	-0.0868	H	-2.4737	0.3121	-0.0868
H	-0.1712	3.4515	0.9281	H	-1.1239	3.1404	1.2955
H	-1.0781	5.4729	0.3339	H	-2.0028	5.1709	0.6905
H	0.1714	-3.4514	-0.9282	H	1.1241	-3.1403	-1.2955
H	1.0782	-5.4729	-0.3339	H	2.0028	-5.1709	-0.6903
120°				**150°**			
C	0.8484	1.0703	-0.2839	C	0.8485	1.0703	-0.2838
C	1.3831	-0.1743	0.0486	C	1.3832	-0.1743	0.0487
C	0.5347	-1.2445	0.3324	C	0.5348	-1.2445	0.3325
C	-0.8483	-1.07	0.2838	C	-0.8482	-1.07	0.2839
C	-1.383	0.1746	-0.0486	C	-1.3829	0.1746	-0.0485
C	-0.5346	1.2448	-0.3325	C	-0.5345	1.2448	-0.3324
C	1.0525	-2.4501	0.6544	C	1.0526	-2.4501	0.6545
C	-1.0525	2.4503	-0.6545	C	-1.0524	2.4503	-0.6544
N	-1.8639	3.1057	0.2324	N	-2.264	2.8331	-0.1447
O	-2.3684	4.2799	-0.0813	O	-2.7685	4.0073	-0.4584
N	1.864	-3.1055	-0.2322	N	2.2642	-2.8328	0.1449
O	2.3684	-4.2799	0.0816	O	2.7685	-4.0072	0.4587
O	-0.7996	2.95	-1.7248	O	-0.4465	3.1907	-1.3921
O	0.7995	-2.9497	1.7248	O	0.4464	-3.1902	1.3921
F	-1.6512	-2.0828	0.5524	F	-1.6511	-2.0828	0.5525
H	1.5174	1.9143	-0.5078	H	1.5175	1.9143	-0.5077
H	2.4737	-0.3119	0.087	H	2.4738	-0.3119	0.0871
H	-2.4737	0.3122	-0.0868	H	-2.4736	0.3122	-0.0867
H	-2.0757	2.687	1.129	H	-2.7717	2.2129	0.4733
H	-2.9267	4.7309	0.5289	H	-3.6022	4.2707	-0.1075
H	2.0759	-2.6869	-1.1289	H	2.772	-2.2128	-0.473
H	2.9267	-4.7309	-0.5286	H	3.6022	-4.2707	0.108
180°				**210°**			
C	0.8486	1.0704	-0.284	C	0.8486	1.0704	-0.2839
C	1.3833	-0.1742	0.0485	C	1.3833	-0.1742	0.0486
C	0.5349	-1.2444	0.3323	C	0.5349	-1.2444	0.3324

C	-0.8481	-1.0699	0.2837	C	-0.8481	-1.0699	0.2838
C	-1.3828	0.1747	-0.0487	C	-1.3828	0.1747	-0.0486
C	-0.5344	1.2449	-0.3326	C	-0.5344	1.2449	-0.3325
C	1.0527	-2.45	0.6543	C	1.0527	-2.45	0.6544
C	-1.0523	2.4504	-0.6546	C	-1.0523	2.4504	-0.6545
N	-2.4098	2.6216	-0.7022	N	-2.2622	2.5279	-1.2905
O	-2.9143	3.7959	-1.0159	O	-2.7667	3.7022	-1.6042
N	2.41	-2.6213	0.7021	N	2.2625	-2.5275	1.2904
O	2.9144	-3.7957	1.0158	O	2.7668	-3.702	1.6041
O	-0.3177	3.3774	-0.9005	O	-0.4479	3.4601	-0.3813
O	0.3178	-3.3768	0.9001	O	0.4481	-3.4594	0.381
F	-1.651	-2.0827	0.5523	F	-1.651	-2.0827	0.5524
H	1.5176	1.9144	-0.5079	H	1.5176	1.9144	-0.5078
H	2.4739	-0.3118	0.0869	H	2.4739	-0.3118	0.087
H	-2.4735	0.3123	-0.0869	H	-2.4735	0.3123	-0.0868
H	-3.0253	1.8451	-0.4963	H	-2.7686	1.6821	-1.5194
H	-3.8484	3.9136	-1.0486	H	-3.5993	3.7554	-2.0417
H	3.0256	-1.8449	0.4962	H	2.7689	-1.6819	1.5194
H	3.8484	-3.9136	1.0486	H	3.5993	-3.7554	2.0417
240°				**270°**			
C	0.8486	1.0704	-0.2838	C	0.8484	1.0704	-0.2837
C	1.3833	-0.1742	0.0487	C	1.3831	-0.1742	0.0488
C	0.5349	-1.2444	0.3325	C	0.5347	-1.2444	0.3326
C	-0.8481	-1.0699	0.2839	C	-0.8483	-1.0699	0.284
C	-1.3828	0.1747	-0.0485	C	-1.383	0.1747	-0.0484
C	-0.5344	1.2449	-0.3324	C	-0.5346	1.2449	-0.3323
C	1.0527	-2.45	0.6545	C	1.0525	-2.45	0.6546
C	-1.0523	2.4504	-0.6544	C	-1.0525	2.4504	-0.6543
N	-1.8608	2.577	-1.752	N	-1.3132	2.7559	-1.9632
O	-2.3652	3.7513	-2.0657	O	-1.8177	3.9302	-2.2769
N	1.861	-2.5767	1.752	N	1.313	-2.7556	1.9633
O	2.3653	-3.7512	2.0657	O	1.8174	-3.9301	2.2769
O	-0.8021	3.4167	0.0261	O	-1.2856	3.2588	0.2125
O	0.8024	-3.4161	-0.0262	O	1.2855	-3.2583	-0.2125
F	-1.651	-2.0827	0.5525	F	-1.6512	-2.0827	0.5526
H	1.5176	1.9144	-0.5077	H	1.5174	1.9144	-0.5076
H	2.4739	-0.3118	0.0871	H	2.4737	-0.3118	0.0872
H	-2.4735	0.3123	-0.0867	H	-2.4737	0.3123	-0.0866
H	-2.0704	1.7676	-2.3221	H	-1.1179	2.0787	-2.6894
H	-2.9216	3.8384	-2.8209	H	-1.9971	4.1403	-3.1774
H	2.0707	-1.7674	2.3222	H	1.1178	-2.0785	2.6896
H	2.9216	-3.8384	2.8209	H	1.9967	-4.1403	3.1774
300°				**330°**			
C	0.8484	1.0703	-0.2837	C	0.8484	1.0703	-0.2837
C	1.3831	-0.1743	0.0488	C	1.3831	-0.1743	0.0488

C	0.5347	-1.2445	0.3326	C	0.5347	-1.2445	0.3326
C	-0.8483	-1.07	0.284	C	-0.8483	-1.07	0.284
C	-1.383	0.1746	-0.0484	C	-1.383	0.1746	-0.0484
C	-0.5346	1.2448	-0.3323	C	-0.5346	1.2448	-0.3323
C	1.0525	-2.4501	0.6546	C	1.0525	-2.4501	0.6546
C	-1.0525	2.4503	-0.6543	C	-1.0525	2.4503	-0.6543
N	-0.7659	3.0165	-1.8674	N	-0.3657	3.2891	-1.4903
O	-1.2704	4.1908	-2.181	O	-0.8702	4.4634	-1.8039
N	0.7658	-3.0163	1.8676	N	0.3656	-3.289	1.4905
O	1.2702	-4.1908	2.1811	O	0.8701	-4.4634	1.804
O	-1.7685	3.0287	0.1281	O	-2.1216	2.7881	-0.2046
O	1.7685	-3.0283	-0.1279	O	2.1216	-2.7879	0.2049
F	-1.6512	-2.0828	0.5526	F	-1.6512	-2.0828	0.5526
H	1.5174	1.9143	-0.5076	H	1.5174	1.9143	-0.5076
H	2.4737	-0.3119	0.0872	H	2.4737	-0.3119	0.0872
H	-2.4737	0.3122	-0.0866	H	-2.4737	0.3122	-0.0866
H	-0.1661	2.5321	-2.5228	H	0.5299	3.0062	-1.867
H	-1.0732	4.5803	-3.0158	H	-0.3976	5.0405	-2.3793
H	0.1659	-2.5319	2.523	H	-0.53	-3.006	1.8672
H	1.0729	-4.5803	3.0158	H	0.3974	-5.0405	2.3793

Table S7 Cartesian coordinates of the H_2-FH-BDHA ligand geometry after counter-rotation of both hydroxamate groups.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.8484	1.3279	0.298
C	1.3831	-0.1744	0.0488	C	1.3831	0.0833	0.6305
C	0.5347	-1.2446	0.3326	C	0.5347	-0.9869	0.9143
C	-0.8483	-1.0701	0.284	C	-0.8483	-0.8124	0.8657
C	-1.383	0.1745	-0.0484	C	-1.383	0.4322	0.5333
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.5024	0.2494
C	1.0525	-2.4502	0.6546	C	1.0525	-2.1925	1.2363
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.7079	-0.0726
N	-0.2198	3.5006	-0.933	N	-0.3657	3.5467	-0.9086
O	-0.7243	4.6749	-1.2466	O	-0.8702	4.721	-1.2222
N	0.2198	-3.5005	0.9331	N	0.3674	-3.3366	0.9266
O	0.7243	-4.6749	1.2467	O	0.8719	-4.5109	1.2402
O	-2.2503	2.6014	-0.6964	O	-2.1216	3.0457	0.3771
O	2.2503	-2.6013	0.6967	O	2.1201	-2.2609	1.7976
F	-1.6512	-2.0829	0.5526	F	-1.6512	-1.8252	1.1343
H	1.5174	1.9142	-0.5076	H	1.5174	2.1719	0.0741
H	2.4737	-0.312	0.0872	H	2.4737	-0.0543	0.6689
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.5698	0.4951
H	0.7836	3.374	-0.8977	H	0.5299	3.2638	-1.2853
H	-0.1513	5.3976	-1.4384	H	-0.3976	5.2981	-1.7976

H	-0.7836	-3.3739	0.8978	H	-0.5269	-3.2792	0.4564
H	0.1513	-5.3976	1.4384	H	0.4005	-5.2981	1.0271
	60°				**90°**		
C	0.8484	1.5165	0.4126	C	0.8484	1.5856	0.4003
C	1.3831	0.2719	0.7451	C	1.3831	0.341	0.7328
C	0.5347	-0.7983	1.0289	C	0.5347	-0.7292	1.0166
C	-0.8483	-0.6238	0.9803	C	-0.8483	-0.5547	0.968
C	-1.383	0.6208	0.6479	C	-1.383	0.6899	0.6356
C	-0.5346	1.691	0.364	C	-0.5346	1.7601	0.3517
C	1.0525	-2.0039	1.3509	C	1.0525	-1.9348	1.3386
C	-1.0525	2.8965	0.042	C	-1.0525	2.9656	0.0297
N	-0.7659	3.4627	-1.1711	N	-1.3132	3.2711	-1.2792
O	-1.2704	4.637	-1.4847	O	-1.8177	4.4454	-1.5929
N	0.7689	-3.0988	0.5796	N	1.3166	-2.8508	0.3561
O	1.2734	-4.2731	0.8933	O	1.8211	-4.0252	0.6698
O	-1.7685	3.4749	0.8244	O	-1.2856	3.774	0.8965
O	1.7658	-2.1157	2.3195	O	1.2824	-2.2044	2.4935
F	-1.6512	-1.6366	1.2489	F	-1.6512	-1.5675	1.2366
H	1.5174	2.3605	0.1887	H	1.5174	2.4296	0.1764
H	2.4737	0.1343	0.7835	H	2.4737	0.2034	0.7712
H	-2.4737	0.7584	0.6097	H	-2.4737	0.8275	0.5974
H	-0.1661	2.9782	-1.8265	H	-1.1179	2.5939	-2.0054
H	-1.0732	5.0265	-2.3195	H	-1.9971	4.6555	-2.4935
H	0.1714	-3.0051	-0.2317	H	1.1241	-2.6249	-0.6114
H	1.0782	-5.0265	0.3626	H	2.0028	-4.6555	-0.0062
	120°				**150°**		
C	0.846	1.5166	0.2642	C	0.8471	1.328	0.0409
C	1.3807	0.272	0.5967	C	1.3818	0.0834	0.3734
C	0.5323	-0.7982	0.8805	C	0.5334	-0.9868	0.6572
C	-0.8507	-0.6237	0.8319	C	-0.8496	-0.8123	0.6086
C	-1.3854	0.6209	0.4995	C	-1.3843	0.4323	0.2762
C	-0.537	1.6911	0.2156	C	-0.5359	1.5025	-0.0077
C	1.0501	-2.0038	1.2025	C	1.0512	-2.1924	0.9792
C	-1.0549	2.8966	-0.1064	C	-1.0538	2.708	-0.3297
N	-1.8634	3.0232	-1.204	N	-2.2638	2.7855	-0.9656
O	-2.3679	4.1975	-1.5177	O	-2.7682	3.9598	-1.2793
N	1.8615	-2.6592	0.3158	N	2.2628	-2.5751	0.4696
O	2.3659	-3.8335	0.6296	O	2.7671	-3.7496	0.7834
O	-0.8047	3.8629	0.5741	O	-0.4494	3.7177	-0.0565
O	0.797	-2.5034	2.2729	O	0.445	-2.9325	1.7168
F	-1.6536	-1.6365	1.1005	F	-1.6525	-1.8251	0.8772
H	1.515	2.3606	0.0403	H	1.5161	2.172	-0.183
H	2.4713	0.1344	0.6351	H	2.4724	-0.0542	0.4118
H	-2.4761	0.7585	0.4613	H	-2.475	0.5699	0.238
H	-2.073	2.2138	-1.7741	H	-2.7701	1.9397	-1.1945

H	-2.9242	4.2845	-2.2729	H	-3.6008	4.013	-1.7168
H	2.0735	-2.2406	-0.5808	H	2.7705	-1.9551	-0.1482
H	2.9242	-4.2845	0.0195	H	3.6008	-4.013	0.4327
	180°				**210°**		
C	0.8486	1.0704	-0.284	C	0.85	0.8127	-0.6087
C	1.3833	-0.1742	0.0485	C	1.3847	-0.4318	-0.2762
C	0.5349	-1.2444	0.3323	C	0.5363	-1.502	0.0076
C	-0.8481	-1.0699	0.2837	C	-0.8467	-1.3275	-0.041
C	-1.3828	0.1747	-0.0487	C	-1.3814	-0.083	-0.3734
C	-0.5344	1.2449	-0.3326	C	-0.533	0.9872	-0.6573
C	1.0527	-2.45	0.6543	C	1.0541	-2.7076	0.3296
C	-1.0523	2.4504	-0.6546	C	-1.0509	2.1927	-0.9793
N	-2.4098	2.6216	-0.7022	N	-2.2625	2.5755	-0.4695
O	-2.9143	3.7959	-1.0159	O	-2.767	3.7497	-0.7832
N	2.41	-2.6213	0.7021	N	2.2639	-2.7852	0.9656
O	2.9144	-3.7957	1.0158	O	2.7682	-3.9597	1.2793
O	-0.3177	3.3774	-0.9005	O	-0.4449	2.9331	-1.7169
O	0.3178	-3.3768	0.9001	O	0.4495	-3.7171	0.0563
F	-1.651	-2.0827	0.5523	F	-1.6496	-2.3403	0.2276
H	1.5176	1.9144	-0.5079	H	1.519	1.6567	-0.8326
H	2.4739	-0.3118	0.0869	H	2.4753	-0.5694	-0.2378
H	-2.4735	0.3123	-0.0869	H	-2.4721	0.0546	-0.4116
H	-3.0253	1.8451	-0.4963	H	-2.7701	1.9553	0.1484
H	-3.8484	3.9136	-1.0486	H	-3.6007	4.0131	-0.4324
H	3.0256	-1.8449	0.4962	H	2.7704	-1.9396	1.1946
H	3.8484	-3.9136	1.0486	H	3.6007	-4.0131	1.7169
	240°				**270°**		
C	0.8511	0.6241	-0.8319	C	0.8484	0.555	-0.9679
C	1.3858	-0.6205	-0.4994	C	1.3831	-0.6896	-0.6354
C	0.5374	-1.6907	-0.2156	C	0.5347	-1.7598	-0.3516
C	-0.8456	-1.5162	-0.2642	C	-0.8483	-1.5853	-0.4002
C	-1.3803	-0.2716	-0.5966	C	-1.383	-0.3407	-0.7326
C	-0.5319	0.7986	-0.8805	C	-0.5346	0.7295	-1.0165
C	1.0552	-2.8963	0.1064	C	1.0525	-2.9654	-0.0296
C	-1.0498	2.0041	-1.2025	C	-1.0525	1.935	-1.3385
N	-1.8612	2.6595	-0.3156	N	-1.3166	2.8511	-0.3559
O	-2.3658	3.8338	-0.6293	O	-1.8211	4.0254	-0.6696
N	1.8635	-3.023	1.204	N	1.313	-3.271	1.2792
O	2.3678	-4.1975	1.5176	O	1.8174	-4.4455	1.5928
O	-0.797	2.5039	-2.2729	O	-1.2826	2.2047	-2.4933
O	0.8048	-3.8624	-0.5742	O	1.2855	-3.7737	-0.8966
F	-1.6485	-2.529	0.0044	F	-1.6512	-2.5981	-0.1316
H	1.5201	1.4681	-1.0558	H	1.5174	1.399	-1.1918
H	2.4764	-0.7581	-0.461	H	2.4737	-0.8272	-0.597
H	-2.471	-0.134	-0.6348	H	-2.4737	-0.2031	-0.7708

H	-2.0731	2.2409	0.581	H	-1.1239	2.6252	0.6115
H	-2.924	4.2847	-0.0191	H	-2.0028	4.6557	0.0065
H	2.0731	-2.2137	1.7742	H	1.1178	-2.5939	2.0055
H	2.924	-4.2847	2.2729	H	1.9967	-4.6557	2.4933
300°				**330°**			
C	0.8484	0.624	-0.9802	C	0.8484	0.8126	-0.8656
C	1.3831	-0.6206	-0.6477	C	1.3831	-0.432	-0.5331
C	0.5347	-1.6908	-0.3639	C	0.5347	-1.5022	-0.2493
C	-0.8483	-1.5163	-0.4125	C	-0.8483	-1.3277	-0.2979
C	-1.383	-0.2717	-0.7449	C	-1.383	-0.0831	-0.6303
C	-0.5346	0.7985	-1.0288	C	-0.5346	0.9871	-0.9142
C	1.0525	-2.8964	-0.0419	C	1.0525	-2.7078	0.0727
C	-1.0525	2.004	-1.3508	C	-1.0525	2.1926	-1.2362
N	-0.7688	3.099	-0.5795	N	-0.3674	3.3367	-0.9265
O	-1.2733	4.2733	-0.8931	O	-0.8719	4.511	-1.2401
N	0.7658	-3.4626	1.171	N	0.3656	-3.5466	0.9086
O	1.2702	-4.6371	1.4846	O	0.8701	-4.7211	1.2221
O	-1.7659	2.1159	-2.3193	O	-2.1201	2.2611	-1.7973
O	1.7685	-3.4747	-0.8244	O	2.1216	-3.0456	-0.377
F	-1.6512	-2.5291	-0.1439	F	-1.6512	-2.3405	-0.0293
H	1.5174	1.468	-1.2041	H	1.5174	1.6566	-1.0895
H	2.4737	-0.7582	-0.6093	H	2.4737	-0.5696	-0.4947
H	-2.4737	-0.1341	-0.7831	H	-2.4737	0.0545	-0.6685
H	-0.1712	3.0053	0.2318	H	0.5269	3.2794	-0.4564
H	-1.0781	5.0267	-0.3624	H	-0.4004	5.2982	-1.0271
H	0.1659	-2.9782	1.8265	H	-0.53	-3.2637	1.2853
H	1.0729	-5.0267	2.3193	H	0.3974	-5.2982	1.7973

Table S8 Cartesian coordinates of the rotated geometry for the hydroxamate group distal to the F side in the H_2-ClH-BDHA ligand.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.8484	1.2488	0.1867
C	1.3831	-0.1744	0.0488	C	1.3831	0.0042	0.5192
C	0.5347	-1.2446	0.3326	C	0.5347	-1.066	0.803
C	-0.8483	-1.0701	0.284	C	-0.8483	-0.8915	0.7544
C	-1.383	0.1745	-0.0484	C	-1.383	0.3531	0.422
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.4233	0.1381
C	1.0525	-2.4502	0.6546	C	1.0525	-2.2716	1.125
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.6288	-0.1839
N	-0.2198	3.5006	-0.933	N	-0.3657	3.4676	-1.0199
O	-0.7243	4.6749	-1.2466	O	-0.8702	4.6419	-1.3335
N	0.2198	-3.5005	0.9331	N	0.2198	-3.3219	1.4035
O	0.7243	-4.6749	1.2467	O	0.7243	-4.4963	1.7171
O	-2.2503	2.6014	-0.6964	O	-2.1216	2.9666	0.2658

O	2.2503	-2.6013	0.6967	O	2.2503	-2.4227	1.1671
Cl	-1.8939	-2.389	0.6338	Cl	-1.8939	-2.2104	1.1042
H	1.5174	1.9142	-0.5076	H	1.5174	2.0928	-0.0372
H	2.4737	-0.312	0.0872	H	2.4737	-0.1334	0.5576
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.4907	0.3838
H	0.7836	3.374	-0.8977	H	0.5299	3.1847	-1.3966
H	-0.1513	5.3976	-1.4384	H	-0.3976	5.219	-1.9088
H	-0.7836	-3.3739	0.8978	H	-0.7836	-3.1953	1.3682
H	0.1513	-5.3976	1.4384	H	0.1513	-5.219	1.9088
	60°				**90°**		
C	0.8484	1.4789	0.505	C	0.8484	1.6989	0.5858
C	1.3831	0.2343	0.8375	C	1.3831	0.4543	0.9183
C	0.5347	-0.8359	1.1213	C	0.5347	-0.6159	1.2021
C	-0.8483	-0.6614	1.0727	C	-0.8483	-0.4414	1.1535
C	-1.383	0.5832	0.7403	C	-1.383	0.8032	0.8211
C	-0.5346	1.6534	0.4564	C	-0.5346	1.8734	0.5372
C	1.0525	-2.0415	1.4433	C	1.0525	-1.8215	1.5241
C	-1.0525	2.8589	0.1344	C	-1.0525	3.0789	0.2152
N	-0.7659	3.4251	-1.0787	N	-1.3132	3.3844	-1.0937
O	-1.2704	4.5994	-1.3924	O	-1.8177	4.5587	-1.4073
N	0.2198	-3.0918	1.7218	N	0.2198	-2.8718	1.8026
O	0.7243	-4.2662	2.0354	O	0.7243	-4.0462	2.1162
O	-1.7685	3.4373	0.9168	O	-1.2856	3.8874	1.0821
O	2.2503	-2.1926	1.4854	O	2.2503	-1.9726	1.5662
Cl	-1.8939	-1.9803	1.4225	Cl	-1.8939	-1.7603	1.5033
H	1.5174	2.3229	0.2811	H	1.5174	2.5429	0.3619
H	2.4737	0.0967	0.8759	H	2.4737	0.3167	0.9567
H	-2.4737	0.7208	0.7021	H	-2.4737	0.9408	0.7829
H	-0.1661	2.9406	-1.7341	H	-1.1179	2.7073	-1.8199
H	-1.0732	4.9889	-2.2271	H	-1.9971	4.7689	-2.3079
H	-0.7836	-2.9652	1.6865	H	-0.7836	-2.7452	1.7673
H	0.1513	-4.9889	2.2271	H	0.1513	-4.7689	2.3079
	120°				**150°**		
C	1.0724	1.8499	0.4075	C	1.4113	1.8914	0.0178
C	1.6071	0.6053	0.74	C	1.946	0.6468	0.3503
C	0.7587	-0.4649	1.0238	C	1.0976	-0.4234	0.6341
C	-0.6243	-0.2904	0.9752	C	-0.2854	-0.2489	0.5855
C	-1.159	0.9542	0.6428	C	-0.8201	0.9957	0.2531
C	-0.3106	2.0244	0.3589	C	0.0283	2.0659	-0.0308
C	1.2765	-1.6705	1.3458	C	1.6154	-1.629	0.9561
C	-0.8285	3.2299	0.0369	C	-0.4896	3.2714	-0.3528
N	-1.637	3.3565	-1.0607	N	-1.6996	3.3489	-0.9887
O	-2.1414	4.5308	-1.3744	O	-2.204	4.5231	-1.3024
N	0.4438	-2.7208	1.6243	N	0.7827	-2.6793	1.2346
O	0.9483	-3.8952	1.9379	O	1.2872	-3.8537	1.5482

O	-0.5783	4.1962	0.7174	O	0.1148	4.2811	-0.0796
O	2.4743	-1.8216	1.3879	O	2.8132	-1.7801	0.9982
Cl	-1.6699	-1.6093	1.325	Cl	-1.331	-1.5678	0.9353
H	1.7414	2.6939	0.1836	H	2.0803	2.7354	-0.2061
H	2.6977	0.4677	0.7784	H	3.0366	0.5092	0.3887
H	-2.2497	1.0918	0.6046	H	-1.9108	1.1333	0.2149
H	-1.8465	2.5471	-1.6308	H	-2.2059	2.5031	-1.2176
H	-2.6977	4.6179	-2.1296	H	-3.0366	4.5764	-1.7399
H	-0.5596	-2.5942	1.589	H	-0.2207	-2.5527	1.1993
H	0.3753	-4.6179	2.1296	H	0.7142	-4.5764	1.7399
180°				**210°**			
C	1.5358	1.8123	-0.4787	C	1.4127	1.6337	-0.3069
C	2.0705	0.5677	-0.1462	C	1.9474	0.3891	0.0256
C	1.2221	-0.5025	0.1376	C	1.099	-0.6811	0.3094
C	-0.1609	-0.328	0.089	C	-0.284	-0.5066	0.2608
C	-0.6956	0.9166	-0.2434	C	-0.8187	0.738	-0.0716
C	0.1528	1.9868	-0.5273	C	0.0297	1.8082	-0.3555
C	1.7399	-1.7081	0.4596	C	1.6168	-1.8867	0.6314
C	-0.3651	3.1923	-0.8493	C	-0.4882	3.0137	-0.6775
N	-1.7226	3.3635	-0.8969	N	-1.6998	3.3965	-0.1677
O	-2.2271	4.5378	-1.2107	O	-2.2043	4.5707	-0.4815
N	0.9072	-2.7584	0.7381	N	0.7841	-2.937	0.9099
O	1.4117	-3.9328	1.0517	O	1.2886	-4.1114	1.2235
O	0.3695	4.1193	-1.0952	O	0.1177	3.7541	-1.4152
O	2.9377	-1.8592	0.5017	O	2.8146	-2.0378	0.6735
Cl	-1.2065	-1.6469	0.4388	Cl	-1.3296	-1.8255	0.6106
H	2.2048	2.6563	-0.7026	H	2.0817	2.4777	-0.5308
H	3.1611	0.4301	-0.1078	H	3.038	0.2515	0.064
H	-1.7863	1.0542	-0.2816	H	-1.9094	0.8756	-0.1098
H	-2.338	2.587	-0.691	H	-2.2075	2.7763	0.4502
H	-3.1611	4.6555	-1.2434	H	-3.038	4.8341	-0.1306
H	-0.0962	-2.6318	0.7028	H	-0.2193	-2.8104	0.8746
H	0.8387	-4.6555	1.2434	H	0.7156	-4.8341	1.4152
240°				**270°**			
C	1.0749	1.4036	-0.1406	C	0.8484	1.1836	-0.0983
C	1.6096	0.159	0.1919	C	1.3831	-0.061	0.2342
C	0.7612	-0.9112	0.4757	C	0.5347	-1.1312	0.518
C	-0.6218	-0.7367	0.4271	C	-0.8483	-0.9567	0.4694
C	-1.1565	0.5079	0.0947	C	-1.383	0.2879	0.137
C	-0.3081	1.5781	-0.1892	C	-0.5346	1.3581	-0.1469
C	1.279	-2.1168	0.7977	C	1.0525	-2.3368	0.84
C	-0.826	2.7836	-0.5112	C	-1.0525	2.5636	-0.4689
N	-1.6374	3.439	0.3757	N	-1.3166	3.4797	0.5136
O	-2.1419	4.6133	0.062	O	-1.8211	4.6539	0.2
N	0.4463	-3.1671	1.0762	N	0.2198	-3.3871	1.1185

O	0.9508	-4.3415	1.3898	O	0.7243	-4.5615	1.4321
O	-0.5732	3.2834	-1.5815	O	-1.2826	2.8333	-1.6238
O	2.4768	-2.2679	0.8398	O	2.2503	-2.4879	0.8821
Cl	-1.6674	-2.0556	0.7769	Cl	-1.8939	-2.2756	0.8192
H	1.7439	2.2476	-0.3645	H	1.5174	2.0276	-0.3222
H	2.7002	0.0214	0.2303	H	2.4737	-0.1986	0.2726
H	-2.2472	0.6455	0.0565	H	-2.4737	0.4255	0.0988
H	-1.8493	3.0204	1.2723	H	-1.1239	3.2537	1.4811
H	-2.7002	5.0642	0.6722	H	-2.0028	5.2842	0.8761
H	-0.5571	-3.0405	1.0409	H	-0.7836	-3.2605	1.0832
H	0.3778	-5.0642	1.5815	H	0.1513	-5.2842	1.6238
300°				**330°**			
C	0.8484	1.0326	-0.1915	C	0.8484	0.9911	-0.3952
C	1.3831	-0.212	0.141	C	1.3831	-0.2535	-0.0627
C	0.5347	-1.2822	0.4248	C	0.5347	-1.3237	0.2211
C	-0.8483	-1.1077	0.3762	C	-0.8483	-1.1492	0.1725
C	-1.383	0.1369	0.0438	C	-1.383	0.0954	-0.1599
C	-0.5346	1.2071	-0.2401	C	-0.5346	1.1656	-0.4438
C	1.0525	-2.4878	0.7468	C	1.0525	-2.5293	0.5431
C	-1.0525	2.4126	-0.5621	C	-1.0525	2.3711	-0.7658
N	-0.7688	3.5076	0.2092	N	-0.3674	3.5152	-0.4561
O	-1.2733	4.6818	-0.1045	O	-0.8719	4.6895	-0.7697
N	0.2198	-3.5381	1.0253	N	0.2198	-3.5796	0.8216
O	0.7243	-4.7125	1.3389	O	0.7243	-4.754	1.1352
O	-1.7659	2.5244	-1.5306	O	-2.1201	2.4396	-1.3269
O	2.2503	-2.6389	0.7889	O	2.2503	-2.6804	0.5852
Cl	-1.8939	-2.4266	0.726	Cl	-1.8939	-2.4681	0.5223
H	1.5174	1.8766	-0.4154	H	1.5174	1.8351	-0.6191
H	2.4737	-0.3496	0.1794	H	2.4737	-0.3911	-0.0243
H	-2.4737	0.2745	0.0056	H	-2.4737	0.233	-0.1981
H	-0.1712	3.4139	1.0205	H	0.5269	3.4579	0.014
H	-1.0781	5.4352	0.4262	H	-0.4004	5.4767	-0.5567
H	-0.7836	-3.4115	0.99	H	-0.7836	-3.453	0.7863
H	0.1513	-5.4352	1.5306	H	0.1513	-5.4767	1.3269

Table S9 Cartesian coordinates of the rotated geometry for the hydroxamate group proximal to the F side in the H_2-ClH-BDHA ligand.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	-0.807	1.267	-0.103
C	1.3831	-0.1744	0.0488	C	0.474	1.373	0.438
C	0.5347	-1.2446	0.3326	C	1.08	0.258	1.019
C	-0.8483	-1.0701	0.284	C	0.405	-0.962	1.058
C	-1.383	0.1745	-0.0484	C	-0.876	-1.068	0.516
C	-0.5346	1.2447	-0.3323	C	-1.482	0.047	-0.064

C	1.0525	-2.4502	0.6546	C	2.321	0.361	1.543
C	-1.0525	2.4502	-0.6543	C	-2.723	-0.056	-0.588
N	-0.2198	3.5006	-0.933	N	-3.318	1.038	-1.158
O	-0.7243	4.6749	-1.2466	O	-4.527	0.938	-1.668
N	0.2198	-3.5005	0.9331	N	3.154	-0.725	1.547
O	0.7243	-4.6749	1.2467	O	4.363	-0.626	2.057
O	-2.2503	2.6014	-0.6964	O	-3.308	-1.112	-0.554
O	2.2503	-2.6013	0.6967	O	2.695	1.411	2.008
Cl	-1.8939	-2.389	0.6338	Cl	1.152	-2.335	1.773
H	1.5174	1.9142	-0.5076	H	-1.285	2.145	-0.561
H	2.4737	-0.312	0.0872	H	1.006	2.335	0.408
H	-2.4737	0.3121	-0.0866	H	-1.409	-2.03	0.547
H	0.7836	3.374	-0.8977	H	-2.829	1.923	-1.186
H	-0.1513	5.3976	-1.4384	H	-4.936	1.69	-2.06
H	-0.7836	-3.3739	0.8978	H	2.84	-1.605	1.157
H	0.1513	-5.3976	1.4384	H	4.936	-1.373	2.06
	60°				**90°**		
C	-0.962	1.267	-0.2955	C	-1.029	1.267	-0.4245
C	0.319	1.373	0.2455	C	0.252	1.373	0.1165
C	0.925	0.258	0.8265	C	0.858	0.258	0.6975
C	0.25	-0.962	0.8655	C	0.183	-0.962	0.7365
C	-1.031	-1.068	0.3235	C	-1.098	-1.068	0.1945
C	-1.637	0.047	-0.2565	C	-1.704	0.047	-0.3855
C	2.166	0.361	1.3505	C	2.099	0.361	1.2215
C	-2.878	-0.056	-0.7805	C	-2.945	-0.056	-0.9095
N	-3.473	1.038	-1.3505	N	-3.54	1.038	-1.4795
O	-4.682	0.938	-1.8605	O	-4.749	0.938	-1.9895
N	3.183	-0.413	0.8585	N	3.195	0.12	0.4375
O	4.391	-0.313	1.3695	O	4.404	0.22	0.9475
O	-3.463	-1.112	-0.7465	O	-3.53	-1.112	-0.8755
O	2.378	1.135	2.2525	O	2.241	0.665	2.3815
Cl	0.997	-2.335	1.5805	Cl	0.93	-2.335	1.4515
H	-1.44	2.145	-0.7535	H	-1.507	2.145	-0.8825
H	0.851	2.335	0.2155	H	0.784	2.335	0.0865
H	-1.564	-2.03	0.3545	H	-1.631	-2.03	0.2255
H	-2.984	1.923	-1.3785	H	-3.051	1.923	-1.5075
H	-5.091	1.69	-2.2525	H	-5.158	1.69	-2.3815
H	3.005	-1.062	0.1025	H	3.076	-0.134	-0.5345
H	5.091	-0.846	1.0315	H	5.158	0.055	0.4085
	120°				**150°**		
C	-0.9905	1.267	-0.4295	C	-0.8565	1.267	-0.309
C	0.2905	1.373	0.1115	C	0.4245	1.373	0.232
C	0.8965	0.258	0.6925	C	1.0305	0.258	0.813
C	0.2215	-0.962	0.7315	C	0.3555	-0.962	0.852
C	-1.0595	-1.068	0.1895	C	-0.9255	-1.068	0.31

C	-1.6655	0.047	-0.3905	C	-1.5315	0.047	-0.27
C	2.1375	0.361	1.2165	C	2.2715	0.361	1.337
C	-2.9065	-0.056	-0.9145	C	-2.7725	-0.056	-0.794
N	-3.5015	1.038	-1.4845	N	-3.3675	1.038	-1.364
O	-4.7105	0.938	-1.9945	O	-4.5765	0.938	-1.874
N	3.1875	0.732	0.4205	N	3.1635	1.259	0.814
O	4.3965	0.832	0.9315	O	4.3715	1.358	1.325
O	-3.4915	-1.112	-0.8805	O	-3.3575	-1.112	-0.76
O	2.3205	0.125	2.3865	O	2.5945	-0.34	2.266
Cl	0.9685	-2.335	1.4465	Cl	1.1025	-2.335	1.567
H	-1.4685	2.145	-0.8875	H	-1.3345	2.145	-0.767
H	0.8225	2.335	0.0815	H	0.9565	2.335	0.202
H	-1.5925	-2.03	0.2205	H	-1.4585	-2.03	0.341
H	-3.0125	1.923	-1.5125	H	-2.8785	1.923	-1.392
H	-5.1195	1.69	-2.3865	H	-4.9855	1.69	-2.266
H	3.0345	0.93	-0.5595	H	2.8925	1.846	0.035
H	5.1195	1.088	0.3845	H	4.9855	1.976	0.965
180°				**210°**			
C	-0.663	1.1935	-0.0955	C	-0.462	1.1995	-0.5445
C	0.618	1.2995	0.4455	C	0.819	1.3055	-0.0035
C	1.224	0.1845	1.0265	C	1.425	0.1905	0.5775
C	0.549	-1.0355	1.0655	C	0.75	-1.0295	0.6165
C	-0.732	-1.1415	0.5235	C	-0.531	-1.1355	0.0745
C	-1.338	-0.0265	-0.0565	C	-1.137	-0.0205	-0.5055
C	2.465	0.2875	1.5505	C	2.666	0.2935	1.1015
C	-2.579	-0.1295	-0.5805	C	-2.378	-0.1235	-1.0295
N	-3.174	0.9645	-1.1505	N	-2.973	0.9705	-1.5995
O	-4.383	0.8645	-1.6605	O	-4.182	0.8705	-2.1095
N	3.127	1.4845	1.5115	N	3.09	1.4835	1.6285
O	4.336	1.5845	2.0225	O	4.299	1.5835	2.1385
O	-3.164	-1.1855	-0.5465	O	-2.963	-1.1795	-0.9955
O	2.99	-0.6775	2.0525	O	3.401	-0.6655	1.1045
Cl	1.296	-2.4085	1.7805	Cl	1.497	-2.4025	1.3315
H	-1.141	2.0715	-0.5535	H	-0.94	2.0775	-1.0025
H	1.15	2.2615	0.4155	H	1.351	2.2675	-0.0335
H	-1.265	-2.1035	0.5545	H	-1.064	-2.0975	0.1055
H	-2.685	1.8495	-1.1785	H	-2.484	1.8555	-1.6275
H	-4.792	1.6165	-2.0525	H	-4.591	1.6225	-2.5015
H	2.688	2.2935	1.0905	H	2.474	2.2865	1.6255
H	4.792	2.4085	1.9965	H	4.591	2.4025	2.5015
240°				**270°**			
C	-0.307	1.267	-0.963	C	-0.24	1.267	-1.2095
C	0.974	1.373	-0.422	C	1.041	1.373	-0.6685
C	1.58	0.258	0.159	C	1.647	0.258	-0.0875
C	0.905	-0.962	0.198	C	0.972	-0.962	-0.0485

C	-0.376	-1.068	-0.344	C	-0.309	-1.068	-0.5905
C	-0.982	0.047	-0.924	C	-0.915	0.047	-1.1705
C	2.821	0.361	0.683	C	2.888	0.361	0.4365
C	-2.223	-0.056	-1.448	C	-2.156	-0.056	-1.6945
N	-2.818	1.038	-2.018	N	-2.751	1.038	-2.2645
O	-4.027	0.938	-2.528	O	-3.96	0.938	-2.7745
N	3.062	1.239	1.705	N	3.049	0.705	1.7515
O	4.27	1.338	2.216	O	4.258	0.805	2.2625
O	-2.808	-1.112	-1.414	O	-2.741	-1.112	-1.6605
O	3.718	-0.322	0.249	O	3.855	0.149	-0.2555
Cl	1.652	-2.335	0.913	Cl	1.719	-2.335	0.6665
H	-0.785	2.145	-1.421	H	-0.718	2.145	-1.6675
H	1.506	2.335	-0.452	H	1.573	2.335	-0.6985
H	-0.909	-2.03	-0.313	H	-0.842	-2.03	-0.5595
H	-2.329	1.923	-2.046	H	-2.262	1.923	-2.2925
H	-4.436	1.69	-2.92	H	-4.369	1.69	-3.1665
H	2.31	1.811	2.069	H	2.239	0.883	2.3305
H	4.436	1.942	2.92	H	4.369	1.042	3.1665
	300°				**330°**		
C	-0.2785	1.267	-1.2195	C	-0.4125	1.267	-0.989
C	1.0025	1.373	-0.6785	C	0.8685	1.373	-0.448
C	1.6085	0.258	-0.0975	C	1.4745	0.258	0.133
C	0.9335	-0.962	-0.0585	C	0.7995	-0.962	0.172
C	-0.3475	-1.068	-0.6005	C	-0.4815	-1.068	-0.37
C	-0.9535	0.047	-1.1805	C	-1.0875	0.047	-0.95
C	2.8495	0.361	0.4265	C	2.7155	0.361	0.657
C	-2.1945	-0.056	-1.7045	C	-2.3285	-0.056	-1.474
N	-2.7895	1.038	-2.2745	N	-2.9235	1.038	-2.044
O	-3.9985	0.938	-2.7845	O	-4.1325	0.938	-2.554
N	3.0565	0.093	1.7525	N	3.0815	-0.433	1.71
O	4.2655	0.193	2.2635	O	4.2895	-0.333	2.221
O	-2.7795	-1.112	-1.6705	O	-2.9135	-1.112	-1.44
O	3.7765	0.689	-0.2755	O	3.5025	1.153	0.196
Cl	1.6805	-2.335	0.6565	Cl	1.5465	-2.335	0.887
H	-0.7565	2.145	-1.6775	H	-0.8905	2.145	-1.447
H	1.5345	2.335	-0.7085	H	1.4005	2.335	-0.478
H	-0.8805	-2.03	-0.5695	H	-1.0145	-2.03	-0.339
H	-2.3005	1.923	-2.3025	H	-2.4345	1.923	-2.072
H	-4.4075	1.69	-3.1765	H	-4.5415	1.69	-2.946
H	2.2795	-0.182	2.3405	H	2.4215	-1.097	2.097
H	4.4075	0.009	3.1765	H	4.5415	-0.88	2.946

Table S10 Cartesian coordinates of the H_2-ClH-BDHA ligand geometry after co-rotation of both hydroxamate groups.

0°				30°			
C	0.8484	1.0702	-0.2837	C	0.8484	1.0702	-0.2839
C	1.3831	-0.1744	0.0488	C	1.3831	-0.1744	0.0486
C	0.5347	-1.2446	0.3326	C	0.5347	-1.2446	0.3324
C	-0.8483	-1.0701	0.284	C	-0.8483	-1.0701	0.2838
C	-1.383	0.1745	-0.0484	C	-1.383	0.1745	-0.0486
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.2447	-0.3325
C	1.0525	-2.4502	0.6546	C	1.0525	-2.4502	0.6544
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.4502	-0.6545
N	-0.2198	3.5006	-0.933	N	-0.3674	3.5943	-0.3448
O	-0.7243	4.6749	-1.2466	O	-0.8719	4.7686	-0.6584
N	0.2198	-3.5005	0.9331	N	0.3674	-3.5943	0.3447
O	0.7243	-4.6749	1.2467	O	0.8719	-4.7686	0.6583
O	-2.2503	2.6014	-0.6964	O	-2.1201	2.5187	-1.2157
O	2.2503	-2.6013	0.6967	O	2.1201	-2.5186	1.2157
Cl	-1.8939	-2.389	0.6338	Cl	-1.8939	-2.389	0.6336
H	1.5174	1.9142	-0.5076	H	1.5174	1.9142	-0.5078
H	2.4737	-0.312	0.0872	H	2.4737	-0.312	0.087
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.3121	-0.0868
H	0.7836	3.374	-0.8977	H	0.5269	3.537	0.1253
H	-0.1513	5.3976	-1.4384	H	-0.4004	5.5558	-0.4454
H	-0.7836	-3.3739	0.8978	H	-0.5269	-3.5369	-0.1255
H	0.1513	-5.3976	1.4384	H	0.4005	-5.5558	0.4452
60°				**90°**			
C	0.8484	1.0702	-0.2839	C	0.8484	1.0702	-0.2839
C	1.3831	-0.1744	0.0486	C	1.3831	-0.1744	0.0486
C	0.5347	-1.2446	0.3324	C	0.5347	-1.2446	0.3324
C	-0.8483	-1.0701	0.2838	C	-0.8483	-1.0701	0.2838
C	-1.383	0.1745	-0.0486	C	-1.383	0.1745	-0.0486
C	-0.5346	1.2447	-0.3325	C	-0.5346	1.2447	-0.3325
C	1.0525	-2.4502	0.6544	C	1.0525	-2.4502	0.6544
C	-1.0525	2.4502	-0.6545	C	-1.0525	2.4502	-0.6545
N	-0.7688	3.5452	0.1168	N	-1.3166	3.3663	0.3281
O	-1.2733	4.7194	-0.1968	O	-1.8211	4.5406	0.0144
N	0.7689	-3.5451	-0.1169	N	1.3166	-3.3662	-0.328
O	1.2734	-4.7195	0.1968	O	1.8211	-4.5406	-0.0143
O	-1.7659	2.562	-1.623	O	-1.2826	2.7199	-1.8093
O	1.7658	-2.562	1.623	O	1.2824	-2.7198	1.8093
Cl	-1.8939	-2.389	0.6336	Cl	-1.8939	-2.389	0.6336
H	1.5174	1.9142	-0.5078	H	1.5174	1.9142	-0.5078
H	2.4737	-0.312	0.087	H	2.4737	-0.312	0.087
H	-2.4737	0.3121	-0.0868	H	-2.4737	0.3121	-0.0868
H	-0.1712	3.4515	0.9281	H	-1.1239	3.1404	1.2955
H	-1.0781	5.4729	0.3339	H	-2.0028	5.1709	0.6905
H	0.1714	-3.4514	-0.9282	H	1.1241	-3.1403	-1.2955

H	1.0782	-5.4729	-0.3339	H	2.0028	-5.1709	-0.6903
	120°				**150°**		
C	0.8484	1.0703	-0.2839	C	0.8485	1.0703	-0.2838
C	1.3831	-0.1743	0.0486	C	1.3832	-0.1743	0.0487
C	0.5347	-1.2445	0.3324	C	0.5348	-1.2445	0.3325
C	-0.8483	-1.07	0.2838	C	-0.8482	-1.07	0.2839
C	-1.383	0.1746	-0.0486	C	-1.3829	0.1746	-0.0485
C	-0.5346	1.2448	-0.3325	C	-0.5345	1.2448	-0.3324
C	1.0525	-2.4501	0.6544	C	1.0526	-2.4501	0.6545
C	-1.0525	2.4503	-0.6545	C	-1.0524	2.4503	-0.6544
N	-1.8639	3.1057	0.2324	N	-2.264	2.8331	-0.1447
O	-2.3684	4.2799	-0.0813	O	-2.7685	4.0073	-0.4584
N	1.864	-3.1055	-0.2322	N	2.2642	-2.8328	0.1449
O	2.3684	-4.2799	0.0816	O	2.7685	-4.0072	0.4587
O	-0.7996	2.95	-1.7248	O	-0.4465	3.1907	-1.3921
O	0.7995	-2.9497	1.7248	O	0.4464	-3.1902	1.3921
Cl	-1.8939	-2.3889	0.6336	Cl	-1.8938	-2.3889	0.6337
H	1.5174	1.9143	-0.5078	H	1.5175	1.9143	-0.5077
H	2.4737	-0.3119	0.087	H	2.4738	-0.3119	0.0871
H	-2.4737	0.3122	-0.0868	H	-2.4736	0.3122	-0.0867
H	-2.0757	2.687	1.129	H	-2.7717	2.2129	0.4733
H	-2.9267	4.7309	0.5289	H	-3.6022	4.2707	-0.1075
H	2.0759	-2.6869	-1.1289	H	2.772	-2.2128	-0.473
H	2.9267	-4.7309	-0.5286	H	3.6022	-4.2707	0.108
	180°				**210°**		
C	0.8486	1.0704	-0.284	C	0.8486	1.0704	-0.2839
C	1.3833	-0.1742	0.0485	C	1.3833	-0.1742	0.0486
C	0.5349	-1.2444	0.3323	C	0.5349	-1.2444	0.3324
C	-0.8481	-1.0699	0.2837	C	-0.8481	-1.0699	0.2838
C	-1.3828	0.1747	-0.0487	C	-1.3828	0.1747	-0.0486
C	-0.5344	1.2449	-0.3326	C	-0.5344	1.2449	-0.3325
C	1.0527	-2.45	0.6543	C	1.0527	-2.45	0.6544
C	-1.0523	2.4504	-0.6546	C	-1.0523	2.4504	-0.6545
N	-2.4098	2.6216	-0.7022	N	-2.2622	2.5279	-1.2905
O	-2.9143	3.7959	-1.0159	O	-2.7667	3.7022	-1.6042
N	2.41	-2.6213	0.7021	N	2.2625	-2.5275	1.2904
O	2.9144	-3.7957	1.0158	O	2.7668	-3.702	1.6041
O	-0.3177	3.3774	-0.9005	O	-0.4479	3.4601	-0.3813
O	0.3178	-3.3768	0.9001	O	0.4481	-3.4594	0.381
Cl	-1.8937	-2.3888	0.6335	Cl	-1.8937	-2.3888	0.6336
H	1.5176	1.9144	-0.5079	H	1.5176	1.9144	-0.5078
H	2.4739	-0.3118	0.0869	H	2.4739	-0.3118	0.087
H	-2.4735	0.3123	-0.0869	H	-2.4735	0.3123	-0.0868
H	-3.0253	1.8451	-0.4963	H	-2.7686	1.6821	-1.5194
H	-3.8484	3.9136	-1.0486	H	-3.5993	3.7554	-2.0417

H	3.0256	-1.8449	0.4962	H	2.7689	-1.6819	1.5194
H	3.8484	-3.9136	1.0486	H	3.5993	-3.7554	2.0417
240°				**270°**			
C	0.8486	1.0704	-0.2838	C	0.8484	1.0704	-0.2837
C	1.3833	-0.1742	0.0487	C	1.3831	-0.1742	0.0488
C	0.5349	-1.2444	0.3325	C	0.5347	-1.2444	0.3326
C	-0.8481	-1.0699	0.2839	C	-0.8483	-1.0699	0.284
C	-1.3828	0.1747	-0.0485	C	-1.383	0.1747	-0.0484
C	-0.5344	1.2449	-0.3324	C	-0.5346	1.2449	-0.3323
C	1.0527	-2.45	0.6545	C	1.0525	-2.45	0.6546
C	-1.0523	2.4504	-0.6544	C	-1.0525	2.4504	-0.6543
N	-1.8608	2.577	-1.752	N	-1.3132	2.7559	-1.9632
O	-2.3652	3.7513	-2.0657	O	-1.8177	3.9302	-2.2769
N	1.861	-2.5767	1.752	N	1.313	-2.7556	1.9633
O	2.3653	-3.7512	2.0657	O	1.8174	-3.9301	2.2769
O	-0.8021	3.4167	0.0261	O	-1.2856	3.2588	0.2125
O	0.8024	-3.4161	-0.0262	O	1.2855	-3.2583	-0.2125
Cl	-1.8937	-2.3888	0.6337	Cl	-1.8939	-2.3888	0.6338
H	1.5176	1.9144	-0.5077	H	1.5174	1.9144	-0.5076
H	2.4739	-0.3118	0.0871	H	2.4737	-0.3118	0.0872
H	-2.4735	0.3123	-0.0867	H	-2.4737	0.3123	-0.0866
H	-2.0704	1.7676	-2.3221	H	-1.1179	2.0787	-2.6894
H	-2.9216	3.8384	-2.8209	H	-1.9971	4.1403	-3.1774
H	2.0707	-1.7674	2.3222	H	1.1178	-2.0785	2.6896
H	2.9216	-3.8384	2.8209	H	1.9967	-4.1403	3.1774
300°				**330°**			
C	0.8484	1.0703	-0.2837	C	0.8484	1.0703	-0.2837
C	1.3831	-0.1743	0.0488	C	1.3831	-0.1743	0.0488
C	0.5347	-1.2445	0.3326	C	0.5347	-1.2445	0.3326
C	-0.8483	-1.07	0.284	C	-0.8483	-1.07	0.284
C	-1.383	0.1746	-0.0484	C	-1.383	0.1746	-0.0484
C	-0.5346	1.2448	-0.3323	C	-0.5346	1.2448	-0.3323
C	1.0525	-2.4501	0.6546	C	1.0525	-2.4501	0.6546
C	-1.0525	2.4503	-0.6543	C	-1.0525	2.4503	-0.6543
N	-0.7659	3.0165	-1.8674	N	-0.3657	3.2891	-1.4903
O	-1.2704	4.1908	-2.181	O	-0.8702	4.4634	-1.8039
N	0.7658	-3.0163	1.8676	N	0.3656	-3.289	1.4905
O	1.2702	-4.1908	2.1811	O	0.8701	-4.4634	1.804
O	-1.7685	3.0287	0.1281	O	-2.1216	2.7881	-0.2046
O	1.7685	-3.0283	-0.1279	O	2.1216	-2.7879	0.2049
Cl	-1.8939	-2.3889	0.6338	Cl	-1.8939	-2.3889	0.6338
H	1.5174	1.9143	-0.5076	H	1.5174	1.9143	-0.5076
H	2.4737	-0.3119	0.0872	H	2.4737	-0.3119	0.0872
H	-2.4737	0.3122	-0.0866	H	-2.4737	0.3122	-0.0866
H	-0.1661	2.5321	-2.5228	H	0.5299	3.0062	-1.867

H	-1.0732	4.5803	-3.0158	H	-0.3976	5.0405	-2.3793
H	0.1659	-2.5319	2.523	H	-0.53	-3.006	1.8672
H	1.0729	-4.5803	3.0158	H	0.3974	-5.0405	2.3793

Table S11 Cartesian coordinates of the H_2-ClH-BDHA ligand geometry after counter-rotation of both hydroxamate groups.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.8484	1.3279	0.298
C	1.3831	-0.1744	0.0488	C	1.3831	0.0833	0.6305
C	0.5347	-1.2446	0.3326	C	0.5347	-0.9869	0.9143
C	-0.8483	-1.0701	0.284	C	-0.8483	-0.8124	0.8657
C	-1.383	0.1745	-0.0484	C	-1.383	0.4322	0.5333
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.5024	0.2494
C	1.0525	-2.4502	0.6546	C	1.0525	-2.1925	1.2363
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.7079	-0.0726
N	-0.2198	3.5006	-0.933	N	-0.3657	3.5467	-0.9086
O	-0.7243	4.6749	-1.2466	O	-0.8701	4.721	-1.2222
N	0.2198	-3.5005	0.9331	N	0.3674	-3.3366	0.9266
O	0.7243	-4.6749	1.2467	O	0.8719	-4.5109	1.2402
O	-2.2503	2.6014	-0.6964	O	-2.1216	3.0457	0.3771
O	2.2503	-2.6013	0.6967	O	2.1201	-2.2609	1.7976
Cl	-1.8939	-2.389	0.6338	Cl	-1.8939	-2.1313	1.2155
H	1.5174	1.9142	-0.5076	H	1.5174	2.1719	0.0741
H	2.4737	-0.312	0.0872	H	2.4737	-0.0543	0.6689
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.5698	0.4951
H	0.7836	3.374	-0.8977	H	0.5299	3.2638	-1.2853
H	-0.1513	5.3976	-1.4384	H	-0.3976	5.2981	-1.7976
H	-0.7836	-3.3739	0.8978	H	-0.5269	-3.2792	0.4564
H	0.1513	-5.3976	1.4384	H	0.4005	-5.2981	1.0271
60°				**90°**			
C	0.8484	1.5165	0.4126	C	0.8484	1.5856	0.4003
C	1.3831	0.2719	0.7451	C	1.3831	0.341	0.7328
C	0.5347	-0.7983	1.0289	C	0.5347	-0.7292	1.0166
C	-0.8483	-0.6238	0.9803	C	-0.8483	-0.5547	0.968
C	-1.383	0.6208	0.6479	C	-1.383	0.6899	0.6356
C	-0.5346	1.691	0.364	C	-0.5346	1.7601	0.3517
C	1.0525	-2.0039	1.3509	C	1.0525	-1.9348	1.3386
C	-1.0525	2.8965	0.042	C	-1.0525	2.9656	0.0297
N	-0.7659	3.4627	-1.1711	N	-1.3132	3.2711	-1.2792
O	-1.2704	4.637	-1.4847	O	-1.8177	4.4454	-1.5929
N	0.7689	-3.0988	0.5796	N	1.3166	-2.8508	0.3561
O	1.2734	-4.2731	0.8933	O	1.8211	-4.0252	0.6698
O	-1.7685	3.4749	0.8244	O	-1.2856	3.774	0.8965
O	1.7658	-2.1157	2.3195	O	1.2824	-2.2044	2.4935

Cl	-1.8939	-1.9427	1.3301	Cl	-1.8939	-1.8736	1.3178
H	1.5174	2.3605	0.1887	H	1.5174	2.4296	0.1764
H	2.4737	0.1343	0.7835	H	2.4737	0.2034	0.7712
H	-2.4737	0.7584	0.6097	H	-2.4737	0.8275	0.5974
H	-0.1661	2.9782	-1.8265	H	-1.1179	2.5939	-2.0054
H	-1.0732	5.0265	-2.3195	H	-1.9971	4.6555	-2.4935
H	0.1714	-3.0051	-0.2317	H	1.1241	-2.6249	-0.6114
H	1.0782	-5.0265	0.3626	H	2.0028	-4.6555	-0.0062
	120°				**150°**		
C	0.846	1.5166	0.2642	C	0.8471	1.328	0.0409
C	1.3807	0.272	0.5967	C	1.3818	0.0834	0.3734
C	0.5323	-0.7982	0.8805	C	0.5334	-0.9868	0.6572
C	-0.8507	-0.6237	0.8319	C	-0.8496	-0.8123	0.6086
C	-1.3854	0.6209	0.4995	C	-1.3843	0.4323	0.2762
C	-0.537	1.6911	0.2156	C	-0.5359	1.5025	-0.0077
C	1.0501	-2.0038	1.2025	C	1.0512	-2.1924	0.9792
C	-1.0549	2.8966	-0.1064	C	-1.0538	2.708	-0.3297
N	-1.8634	3.0232	-1.204	N	-2.2638	2.7855	-0.9656
O	-2.3679	4.1975	-1.5177	O	-2.7682	3.9598	-1.2793
N	1.8615	-2.6592	0.3158	N	2.2628	-2.5751	0.4696
O	2.3659	-3.8335	0.6296	O	2.7671	-3.7496	0.7834
O	-0.8047	3.8629	0.5741	O	-0.4494	3.7177	-0.0565
O	0.797	-2.5034	2.2729	O	0.445	-2.9325	1.7168
Cl	-1.8963	-1.9426	1.1817	Cl	-1.8952	-2.1312	0.9584
H	1.515	2.3606	0.0403	H	1.5161	2.172	-0.183
H	2.4713	0.1344	0.6351	H	2.4724	-0.0542	0.4118
H	-2.4761	0.7585	0.4613	H	-2.475	0.5699	0.238
H	-2.073	2.2138	-1.7741	H	-2.7701	1.9397	-1.1945
H	-2.9242	4.2845	-2.2729	H	-3.6008	4.013	-1.7168
H	2.0735	-2.2406	-0.5808	H	2.7705	-1.9551	-0.1482
H	2.9242	-4.2845	0.0195	H	3.6008	-4.013	0.4327
	180°				**210°**		
C	0.8486	1.0704	-0.284	C	0.85	0.8127	-0.6087
C	1.3833	-0.1742	0.0485	C	1.3847	-0.4318	-0.2762
C	0.5349	-1.2444	0.3323	C	0.5363	-1.502	0.0076
C	-0.8481	-1.0699	0.2837	C	-0.8467	-1.3275	-0.041
C	-1.3828	0.1747	-0.0487	C	-1.3814	-0.083	-0.3734
C	-0.5344	1.2449	-0.3326	C	-0.533	0.9872	-0.6573
C	1.0527	-2.45	0.6543	C	1.0541	-2.7076	0.3296
C	-1.0523	2.4504	-0.6546	C	-1.0509	2.1927	-0.9793
N	-2.4098	2.6216	-0.7022	N	-2.2625	2.5755	-0.4695
O	-2.9143	3.7959	-1.0159	O	-2.767	3.7497	-0.7832
N	2.41	-2.6213	0.7021	N	2.2639	-2.7852	0.9656
O	2.9144	-3.7957	1.0158	O	2.7682	-3.9597	1.2793
O	-0.3177	3.3774	-0.9005	O	-0.4449	2.9331	-1.7169

O	0.3178	-3.3768	0.9001	O	0.4495	-3.7171	0.0563
Cl	-1.8937	-2.3888	0.6335	Cl	-1.8923	-2.6464	0.3088
H	1.5176	1.9144	-0.5079	H	1.519	1.6567	-0.8326
H	2.4739	-0.3118	0.0869	H	2.4753	-0.5694	-0.2378
H	-2.4735	0.3123	-0.0869	H	-2.4721	0.0546	-0.4116
H	-3.0253	1.8451	-0.4963	H	-2.7701	1.9553	0.1484
H	-3.8484	3.9136	-1.0486	H	-3.6007	4.0131	-0.4324
H	3.0256	-1.8449	0.4962	H	2.7704	-1.9396	1.1946
H	3.8484	-3.9136	1.0486	H	3.6007	-4.0131	1.7169
240°				**270°**			
C	0.8511	0.6241	-0.8319	C	0.8484	0.555	-0.9679
C	1.3858	-0.6205	-0.4994	C	1.3831	-0.6896	-0.6354
C	0.5374	-1.6907	-0.2156	C	0.5347	-1.7598	-0.3516
C	-0.8456	-1.5162	-0.2642	C	-0.8483	-1.5853	-0.4002
C	-1.3803	-0.2716	-0.5966	C	-1.383	-0.3407	-0.7326
C	-0.5319	0.7986	-0.8805	C	-0.5346	0.7295	-1.0165
C	1.0552	-2.8963	0.1064	C	1.0525	-2.9654	-0.0296
C	-1.0498	2.0041	-1.2025	C	-1.0525	1.935	-1.3385
N	-1.8612	2.6595	-0.3156	N	-1.3166	2.8511	-0.3559
O	-2.3658	3.8338	-0.6293	O	-1.8211	4.0254	-0.6696
N	1.8635	-3.023	1.204	N	1.313	-3.271	1.2792
O	2.3678	-4.1975	1.5176	O	1.8174	-4.4455	1.5928
O	-0.797	2.5039	-2.2729	O	-1.2826	2.2047	-2.4933
O	0.8048	-3.8624	-0.5742	O	1.2855	-3.7737	-0.8966
Cl	-1.8912	-2.8351	0.0856	Cl	-1.8939	-2.9042	-0.0504
H	1.5201	1.4681	-1.0558	H	1.5174	1.399	-1.1918
H	2.4764	-0.7581	-0.461	H	2.4737	-0.8272	-0.597
H	-2.471	-0.134	-0.6348	H	-2.4737	-0.2031	-0.7708
H	-2.0731	2.2409	0.581	H	-1.1239	2.6252	0.6115
H	-2.924	4.2847	-0.0191	H	-2.0028	4.6557	0.0065
H	2.0731	-2.2137	1.7742	H	1.1178	-2.5939	2.0055
H	2.924	-4.2847	2.2729	H	1.9967	-4.6557	2.4933
300°				**330°**			
C	0.8484	0.624	-0.9802	C	0.8484	0.8126	-0.8656
C	1.3831	-0.6206	-0.6477	C	1.3831	-0.432	-0.5331
C	0.5347	-1.6908	-0.3639	C	0.5347	-1.5022	-0.2493
C	-0.8483	-1.5163	-0.4125	C	-0.8483	-1.3277	-0.2979
C	-1.383	-0.2717	-0.7449	C	-1.383	-0.0831	-0.6303
C	-0.5346	0.7985	-1.0288	C	-0.5346	0.9871	-0.9142
C	1.0525	-2.8964	-0.0419	C	1.0525	-2.7078	0.0727
C	-1.0525	2.004	-1.3508	C	-1.0525	2.1926	-1.2362
N	-0.7688	3.099	-0.5795	N	-0.3674	3.3367	-0.9265
O	-1.2733	4.2733	-0.8931	O	-0.8719	4.511	-1.2401
N	0.7658	-3.4626	1.171	N	0.3656	-3.5466	0.9086
O	1.2702	-4.6371	1.4846	O	0.8701	-4.7211	1.2221

O	-1.7659	2.1159	-2.3193	O	-2.1201	2.2611	-1.7974
O	1.7685	-3.4747	-0.8244	O	2.1216	-3.0456	-0.377
Cl	-1.8939	-2.8352	-0.0627	Cl	-1.8939	-2.6466	0.0519
H	1.5174	1.468	-1.2041	H	1.5174	1.6566	-1.0895
H	2.4737	-0.7582	-0.6093	H	2.4737	-0.5696	-0.4947
H	-2.4737	-0.1341	-0.7831	H	-2.4737	0.0545	-0.6685
H	-0.1712	3.0053	0.2318	H	0.5269	3.2794	-0.4564
H	-1.0781	5.0267	-0.3624	H	-0.4004	5.2982	-1.0271
H	0.1659	-2.9782	1.8265	H	-0.53	-3.2637	1.2853
H	1.0729	-5.0267	2.3193	H	0.3974	-5.2982	1.7974

Table S12 Cartesian coordinates of the rotated geometry for the hydroxamate group distal to the F side in the H_2-BrH-BDHA ligand.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.8484	1.2488	0.1867
C	1.3831	-0.1744	0.0488	C	1.3831	0.0042	0.5192
C	0.5347	-1.2446	0.3326	C	0.5347	-1.066	0.803
C	-0.8483	-1.0701	0.284	C	-0.8483	-0.8915	0.7544
C	-1.383	0.1745	-0.0484	C	-1.383	0.3531	0.422
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.4233	0.1381
C	1.0525	-2.4502	0.6546	C	1.0525	-2.2716	1.125
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.6288	-0.1839
N	-0.2198	3.5006	-0.933	N	-0.3657	3.4676	-1.0199
O	-0.7243	4.6749	-1.2466	O	-0.8702	4.6419	-1.3335
N	0.2198	-3.5005	0.9331	N	0.2198	-3.3219	1.4035
O	0.7243	-4.6749	1.2467	O	0.7243	-4.4963	1.7171
O	-2.2503	2.6014	-0.6964	O	-2.1216	2.9666	0.2658
O	2.2503	-2.6013	0.6967	O	2.2503	-2.4227	1.1671
Br	-1.9924	-2.5133	0.6668	Br	-1.9924	-2.3347	1.1372
H	1.5174	1.9142	-0.5076	H	1.5174	2.0928	-0.0372
H	2.4737	-0.312	0.0872	H	2.4737	-0.1334	0.5576
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.4907	0.3838
H	0.7836	3.374	-0.8977	H	0.5299	3.1847	-1.3966
H	-0.1513	5.3976	-1.4384	H	-0.3976	5.219	-1.9088
H	-0.7836	-3.3739	0.8978	H	-0.7836	-3.1953	1.3682
H	0.1513	-5.3976	1.4384	H	0.1513	-5.219	1.9088
60°				**90°**			
C	0.8484	1.4789	0.505	C	0.8484	1.6989	0.5858
C	1.3831	0.2343	0.8375	C	1.3831	0.4543	0.9183
C	0.5347	-0.8359	1.1213	C	0.5347	-0.6159	1.2021
C	-0.8483	-0.6614	1.0727	C	-0.8483	-0.4414	1.1535
C	-1.383	0.5832	0.7403	C	-1.383	0.8032	0.8211
C	-0.5346	1.6534	0.4564	C	-0.5346	1.8734	0.5372
C	1.0525	-2.0415	1.4433	C	1.0525	-1.8215	1.5241

C	-1.0525	2.8589	0.1344	C	-1.0525	3.0789	0.2152
N	-0.7659	3.4251	-1.0787	N	-1.3132	3.3844	-1.0937
O	-1.2704	4.5994	-1.3924	O	-1.8177	4.5587	-1.4073
N	0.2198	-3.0918	1.7218	N	0.2198	-2.8718	1.8026
O	0.7243	-4.2662	2.0354	O	0.7243	-4.0462	2.1162
O	-1.7685	3.4373	0.9168	O	-1.2856	3.8874	1.0821
O	2.2503	-2.1926	1.4854	O	2.2503	-1.9726	1.5662
Br	-1.9924	-2.1046	1.4555	Br	-1.9924	-1.8846	1.5363
H	1.5174	2.3229	0.2811	H	1.5174	2.5429	0.3619
H	2.4737	0.0967	0.8759	H	2.4737	0.3167	0.9567
H	-2.4737	0.7208	0.7021	H	-2.4737	0.9408	0.7829
H	-0.1661	2.9406	-1.7341	H	-1.1179	2.7073	-1.8199
H	-1.0732	4.9889	-2.2271	H	-1.9971	4.7689	-2.3079
H	-0.7836	-2.9652	1.6865	H	-0.7836	-2.7452	1.7673
H	0.1513	-4.9889	2.2271	H	0.1513	-4.7689	2.3079
120°				**150°**			
C	1.0724	1.8499	0.4075	C	1.4113	1.8914	0.0178
C	1.6071	0.6053	0.74	C	1.946	0.6468	0.3503
C	0.7587	-0.4649	1.0238	C	1.0976	-0.4234	0.6341
C	-0.6243	-0.2904	0.9752	C	-0.2854	-0.2489	0.5855
C	-1.159	0.9542	0.6428	C	-0.8201	0.9957	0.2531
C	-0.3106	2.0244	0.3589	C	0.0283	2.0659	-0.0308
C	1.2765	-1.6705	1.3458	C	1.6154	-1.629	0.9561
C	-0.8285	3.2299	0.0369	C	-0.4896	3.2714	-0.3528
N	-1.637	3.3565	-1.0607	N	-1.6996	3.3489	-0.9887
O	-2.1414	4.5308	-1.3744	O	-2.204	4.5231	-1.3024
N	0.4438	-2.7208	1.6243	N	0.7827	-2.6793	1.2346
O	0.9483	-3.8952	1.9379	O	1.2872	-3.8537	1.5482
O	-0.5783	4.1962	0.7174	O	0.1148	4.2811	-0.0796
O	2.4743	-1.8216	1.3879	O	2.8132	-1.7801	0.9982
Br	-1.7684	-1.7336	1.358	Br	-1.4295	-1.6921	0.9683
H	1.7414	2.6939	0.1836	H	2.0803	2.7354	-0.2061
H	2.6977	0.4677	0.7784	H	3.0366	0.5092	0.3887
H	-2.2497	1.0918	0.6046	H	-1.9108	1.1333	0.2149
H	-1.8465	2.5471	-1.6308	H	-2.2059	2.5031	-1.2176
H	-2.6977	4.6179	-2.1296	H	-3.0366	4.5764	-1.7399
H	-0.5596	-2.5942	1.589	H	-0.2207	-2.5527	1.1993
H	0.3753	-4.6179	2.1296	H	0.7142	-4.5764	1.7399
180°				**210°**			
C	1.5358	1.8123	-0.4787	C	1.4127	1.6337	-0.3069
C	2.0705	0.5677	-0.1462	C	1.9474	0.3891	0.0256
C	1.2221	-0.5025	0.1376	C	1.099	-0.6811	0.3094
C	-0.1609	-0.328	0.089	C	-0.284	-0.5066	0.2608
C	-0.6956	0.9166	-0.2434	C	-0.8187	0.738	-0.0716
C	0.1528	1.9868	-0.5273	C	0.0297	1.8082	-0.3555

C	1.7399	-1.7081	0.4596	C	1.6168	-1.8867	0.6314
C	-0.3651	3.1923	-0.8493	C	-0.4882	3.0137	-0.6775
N	-1.7226	3.3635	-0.8969	N	-1.6998	3.3965	-0.1677
O	-2.2271	4.5378	-1.2107	O	-2.2043	4.5707	-0.4815
N	0.9072	-2.7584	0.7381	N	0.7841	-2.937	0.9099
O	1.4117	-3.9328	1.0517	O	1.2886	-4.1114	1.2235
O	0.3695	4.1193	-1.0952	O	0.1177	3.7541	-1.4152
O	2.9377	-1.8592	0.5017	O	2.8146	-2.0378	0.6735
Br	-1.305	-1.7712	0.4718	Br	-1.4281	-1.9498	0.6436
H	2.2048	2.6563	-0.7026	H	2.0817	2.4777	-0.5308
H	3.1611	0.4301	-0.1078	H	3.038	0.2515	0.064
H	-1.7863	1.0542	-0.2816	H	-1.9094	0.8756	-0.1098
H	-2.338	2.587	-0.691	H	-2.2075	2.7763	0.4502
H	-3.1611	4.6555	-1.2434	H	-3.038	4.8341	-0.1306
H	-0.0962	-2.6318	0.7028	H	-0.2193	-2.8104	0.8746
H	0.8387	-4.6555	1.2434	H	0.7156	-4.8341	1.4152
240°				**270°**			
C	1.0749	1.4036	-0.1406	C	0.8484	1.1836	-0.0983
C	1.6096	0.159	0.1919	C	1.3831	-0.061	0.2342
C	0.7612	-0.9112	0.4757	C	0.5347	-1.1312	0.518
C	-0.6218	-0.7367	0.4271	C	-0.8483	-0.9567	0.4694
C	-1.1565	0.5079	0.0947	C	-1.383	0.2879	0.137
C	-0.3081	1.5781	-0.1892	C	-0.5346	1.3581	-0.1469
C	1.279	-2.1168	0.7977	C	1.0525	-2.3368	0.84
C	-0.826	2.7836	-0.5112	C	-1.0525	2.5636	-0.4689
N	-1.6374	3.439	0.3757	N	-1.3166	3.4797	0.5136
O	-2.1419	4.6133	0.062	O	-1.8211	4.6539	0.2
N	0.4463	-3.1671	1.0762	N	0.2198	-3.3871	1.1185
O	0.9508	-4.3415	1.3898	O	0.7243	-4.5615	1.4321
O	-0.5732	3.2834	-1.5815	O	-1.2826	2.8333	-1.6238
O	2.4768	-2.2679	0.8398	O	2.2503	-2.4879	0.8821
Br	-1.7659	-2.1799	0.8099	Br	-1.9924	-2.3999	0.8522
H	1.7439	2.2476	-0.3645	H	1.5174	2.0276	-0.3222
H	2.7002	0.0214	0.2303	H	2.4737	-0.1986	0.2726
H	-2.2472	0.6455	0.0565	H	-2.4737	0.4255	0.0988
H	-1.8493	3.0204	1.2723	H	-1.1239	3.2537	1.4811
H	-2.7002	5.0642	0.6722	H	-2.0028	5.2842	0.8761
H	-0.5571	-3.0405	1.0409	H	-0.7836	-3.2605	1.0832
H	0.3778	-5.0642	1.5815	H	0.1513	-5.2842	1.6238
300°				**330°**			
C	0.8484	1.0326	-0.1915	C	0.8484	0.9911	-0.3952
C	1.3831	-0.212	0.141	C	1.3831	-0.2535	-0.0627
C	0.5347	-1.2822	0.4248	C	0.5347	-1.3237	0.2211
C	-0.8483	-1.1077	0.3762	C	-0.8483	-1.1492	0.1725
C	-1.383	0.1369	0.0438	C	-1.383	0.0954	-0.1599

C	-0.5346	1.2071	-0.2401	C	-0.5346	1.1656	-0.4438
C	1.0525	-2.4878	0.7468	C	1.0525	-2.5293	0.5431
C	-1.0525	2.4126	-0.5621	C	-1.0525	2.3711	-0.7658
N	-0.7688	3.5076	0.2092	N	-0.3674	3.5152	-0.4561
O	-1.2733	4.6818	-0.1045	O	-0.8719	4.6895	-0.7697
N	0.2198	-3.5381	1.0253	N	0.2198	-3.5796	0.8216
O	0.7243	-4.7125	1.3389	O	0.7243	-4.754	1.1352
O	-1.7659	2.5244	-1.5306	O	-2.1201	2.4396	-1.3269
O	2.2503	-2.6389	0.7889	O	2.2503	-2.6804	0.5852
Br	-1.9924	-2.5509	0.759	Br	-1.9924	-2.5924	0.5553
H	1.5174	1.8766	-0.4154	H	1.5174	1.8351	-0.6191
H	2.4737	-0.3496	0.1794	H	2.4737	-0.3911	-0.0243
H	-2.4737	0.2745	0.0056	H	-2.4737	0.233	-0.1981
H	-0.1712	3.4139	1.0205	H	0.5269	3.4579	0.014
H	-1.0781	5.4352	0.4262	H	-0.4004	5.4767	-0.5567
H	-0.7836	-3.4115	0.99	H	-0.7836	-3.453	0.7863
H	0.1513	-5.4352	1.5306	H	0.1513	-5.4767	1.3269

Table S13 Cartesian coordinates of the rotated geometry for the hydroxamate group proximal to the F side in the H_2-BrH-BDHA ligand.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.3715	-0.164	1.323
C	1.3831	-0.1744	0.0488	C	-0.1945	-1.29	0.725
C	0.5347	-1.2446	0.3326	C	-1.0245	-1.145	-0.387
C	-0.8483	-1.0701	0.284	C	-1.2885	0.124	-0.9
C	-1.383	0.1745	-0.0484	C	-0.7225	1.25	-0.302
C	-0.5346	1.2447	-0.3323	C	0.1075	1.106	0.81
C	1.0525	-2.4502	0.6546	C	-1.5725	-2.236	-0.967
C	-1.0525	2.4502	-0.6543	C	0.6565	2.196	1.389
N	-0.2198	3.5006	-0.933	N	1.4705	2.055	2.48
O	-0.7243	4.6749	-1.2466	O	2.0045	3.117	3.045
N	0.2198	-3.5005	0.9331	N	-1.8445	-2.234	-2.308
O	0.7243	-4.6749	1.2467	O	-2.3785	-3.296	-2.873
O	-2.2503	2.6014	-0.6964	O	0.4275	3.296	0.945
O	2.2503	-2.6013	0.6967	O	-1.8235	-3.212	-0.301
Br	-1.9924	-2.5133	0.6668	Br	-2.4075	0.319	-2.4
H	1.5174	1.9142	-0.5076	H	1.0265	-0.278	2.2
H	2.4737	-0.312	0.0872	H	0.0135	-2.291	1.13
H	-2.4737	0.3121	-0.0866	H	-0.9305	2.251	-0.707
H	0.7836	3.374	-0.8977	H	1.6625	1.133	2.853
H	-0.1513	5.3976	-1.4384	H	2.5655	3.019	3.796
H	-0.7836	-3.3739	0.8978	H	-1.6345	-1.416	-2.866
H	0.1513	-5.3976	1.4384	H	-2.5655	-3.295	-3.796
60°				**90°**			

C	0.2925	0.0785	1.2975	C	0.413	0.382	1.0415
C	-0.2735	-1.0475	0.6995	C	-0.153	-0.744	0.4435
C	-1.1035	-0.9025	-0.4125	C	-0.983	-0.599	-0.6685
C	-1.3675	0.3665	-0.9255	C	-1.247	0.67	-1.1815
C	-0.8015	1.4925	-0.3275	C	-0.681	1.796	-0.5835
C	0.0285	1.3485	0.7845	C	0.149	1.652	0.5285
C	-1.6515	-1.9935	-0.9925	C	-1.531	-1.69	-1.2485
C	0.5775	2.4385	1.3635	C	0.698	2.742	1.1075
N	1.3915	2.2975	2.4545	N	1.512	2.601	2.1985
O	1.9255	3.3595	3.0195	O	2.046	3.663	2.7635
N	-1.3825	-2.2795	-2.3035	N	-0.868	-2.336	-2.2565
O	-1.9165	-3.3415	-2.8685	O	-1.402	-3.398	-2.8215
O	0.3485	3.5385	0.9195	O	0.469	3.842	0.6635
O	-2.3795	-2.7155	-0.3535	O	-2.607	-2.095	-0.8765
Br	-2.4865	0.5615	-2.4255	Br	-2.366	0.865	-2.6815
H	0.9475	-0.0355	2.1745	H	1.068	0.268	1.9185
H	-0.0655	-2.0485	1.1045	H	0.055	-1.745	0.8485
H	-1.0095	2.4935	-0.7325	H	-0.889	2.797	-0.9885
H	1.5835	1.3755	2.8275	H	1.704	1.679	2.5715
H	2.4865	3.2615	3.7705	H	2.607	3.565	3.5145
H	-0.7725	-1.6745	-2.8385	H	0.034	-1.996	-2.5675
H	-1.7315	-3.5385	-3.7705	H	-0.945	-3.842	-3.5145
120°				**150°**			
C	0.4755	0.664	0.625	C	0.4105	0.8495	0.625
C	-0.0905	-0.462	0.027	C	-0.1555	-0.2765	0.027
C	-0.9205	-0.317	-1.085	C	-0.9855	-0.1315	-1.085
C	-1.1845	0.952	-1.598	C	-1.2495	1.1375	-1.598
C	-0.6185	2.078	-1	C	-0.6835	2.2635	-1
C	0.2115	1.934	0.112	C	0.1465	2.1195	0.112
C	-1.4685	-1.408	-1.665	C	-1.5335	-1.2225	-1.665
C	0.7605	3.024	0.691	C	0.6955	3.2095	0.691
N	1.5745	2.883	1.782	N	1.5095	3.0685	1.782
O	2.1085	3.945	2.347	O	2.0435	4.1305	2.347
N	-0.6625	-2.388	-2.178	N	-0.8765	-2.4225	-1.625
O	-1.1965	-3.45	-2.743	O	-1.4105	-3.4845	-2.19
O	0.5315	4.124	0.247	O	0.4665	4.3095	0.247
O	-2.6695	-1.518	-1.729	O	-2.6045	-1.1385	-2.218
Br	-2.3035	1.147	-3.098	Br	-2.3685	1.3325	-3.098
H	1.1305	0.55	1.502	H	1.0655	0.7355	1.502
H	0.1175	-1.463	0.432	H	0.0525	-1.2775	0.432
H	-0.8265	3.079	-1.405	H	-0.8915	3.2645	-1.405
H	1.7665	1.961	2.155	H	1.7015	2.1465	2.155
H	2.6695	3.847	3.098	H	2.6045	4.0325	3.098
H	0.3435	-2.296	-2.124	H	0.0205	-2.4925	-1.161
H	-0.6425	-4.124	-3.097	H	-0.9575	-4.3095	-2.162

180°				210°			
C	0.2925	0.889	0.625	C	0.3815	0.771	0.625
C	-0.2735	-0.237	0.027	C	-0.1845	-0.355	0.027
C	-1.1035	-0.092	-1.085	C	-1.0145	-0.21	-1.085
C	-1.3675	1.177	-1.598	C	-1.2785	1.059	-1.598
C	-0.8015	2.303	-1	C	-0.7125	2.185	-1
C	0.0285	2.159	0.112	C	0.1175	2.041	0.112
C	-1.6515	-1.183	-1.665	C	-1.5625	-1.301	-1.665
C	0.5775	3.249	0.691	C	0.6665	3.131	0.691
N	1.3915	3.108	1.782	N	1.4805	2.99	1.782
O	1.9255	4.17	2.347	O	2.0145	4.052	2.347
N	-1.3925	-2.429	-1.161	N	-1.8465	-2.407	-0.91
O	-1.9265	-3.491	-1.725	O	-2.3805	-3.469	-1.475
O	0.3485	4.349	0.247	O	0.4375	4.231	0.247
O	-2.3705	-1.058	-2.628	O	-1.8025	-1.299	-2.849
Br	-2.4865	1.372	-3.098	Br	-2.3975	1.254	-3.098
H	0.9475	0.775	1.502	H	1.0365	0.657	1.502
H	-0.0655	-1.238	0.432	H	0.0235	-1.356	0.432
H	-1.0095	3.304	-1.405	H	-0.9205	3.186	-1.405
H	1.5835	2.186	2.155	H	1.6725	2.068	2.155
H	2.4865	4.072	3.098	H	2.5755	3.954	3.098
H	-0.7905	-2.534	-0.354	H	-1.6455	-2.409	0.082
H	-1.7485	-4.349	-1.379	H	-2.5755	-4.231	-0.956
240°				**270°**			
C	0.838	0.5275	0.625	C	1.171	0.2245	0.625
C	0.272	-0.5985	0.027	C	0.605	-0.9015	0.027
C	-0.558	-0.4535	-1.085	C	-0.225	-0.7565	-1.085
C	-0.822	0.8155	-1.598	C	-0.489	0.5125	-1.598
C	-0.256	1.9415	-1	C	0.077	1.6385	-1
C	0.574	1.7975	0.112	C	0.907	1.4945	0.112
C	-1.106	-1.5445	-1.665	C	-0.773	-1.8475	-1.665
C	1.123	2.8875	0.691	C	1.456	2.5845	0.691
N	1.937	2.7465	1.782	N	2.27	2.4435	1.782
O	2.471	3.8085	2.347	O	2.804	3.5055	2.347
N	-1.931	-2.3625	-0.941	N	-1.992	-2.3065	-1.244
O	-2.465	-3.4245	-1.505	O	-2.526	-3.3685	-1.808
O	0.894	3.9875	0.247	O	1.227	3.6845	0.247
O	-0.869	-1.7965	-2.822	O	-0.188	-2.4175	-2.554
Br	-1.941	1.0105	-3.098	Br	-1.608	0.7075	-3.098
H	1.493	0.4135	1.502	H	1.826	0.1105	1.502
H	0.48	-1.5995	0.432	H	0.813	-1.9025	0.432
H	-0.464	2.9425	-1.405	H	-0.131	2.6395	-1.405
H	2.129	1.8245	2.155	H	2.462	1.5215	2.155
H	3.032	3.7105	3.098	H	3.365	3.4075	3.098
H	-2.13	-2.1505	0.029	H	-2.483	-1.8285	-0.498

H	-3.032	-3.9875	-1.007	H	-3.365	-3.6845	-1.518
	300°				**330°**		
C	1.291	-0.058	0.625	C	1.166	-0.1645	0.72
C	0.725	-1.184	0.027	C	0.6	-1.2905	0.122
C	-0.105	-1.039	-1.085	C	-0.23	-1.1455	-0.99
C	-0.369	0.23	-1.598	C	-0.494	0.1235	-1.503
C	0.197	1.356	-1	C	0.072	1.2495	-0.905
C	1.027	1.212	0.112	C	0.902	1.1055	0.207
C	-0.653	-2.13	-1.665	C	-0.778	-2.2365	-1.57
C	1.576	2.302	0.691	C	1.451	2.1955	0.786
N	2.39	2.161	1.782	N	2.265	2.0545	1.877
O	2.924	3.223	2.347	O	2.799	3.1165	2.442
N	-2.015	-2.254	-1.738	N	-1.991	-2.1405	-2.197
O	-2.549	-3.316	-2.303	O	-2.525	-3.2025	-2.761
O	1.347	3.402	0.247	O	1.222	3.2955	0.342
O	0.058	-2.995	-2.118	O	-0.198	-3.2955	-1.535
Br	-1.488	0.425	-3.098	Br	-1.613	0.3185	-3.003
H	1.946	-0.172	1.502	H	1.821	-0.2785	1.597
H	0.933	-2.185	0.432	H	0.808	-2.2915	0.527
H	-0.011	2.357	-1.405	H	-0.136	2.2505	-1.31
H	2.582	1.239	2.155	H	2.457	1.1325	2.25
H	3.485	3.125	3.098	H	3.36	3.0185	3.193
H	-2.61	-1.53	-1.358	H	-2.478	-1.2535	-2.226
H	-3.485	-3.402	-2.353	H	-3.36	-3.1375	-3.193

Table S14 Cartesian coordinates of the H_2-BrH-BDHA ligand geometry after co-rotation of both hydroxamate groups.

	0°				**30°**		
C	0.8484	1.0702	-0.2837	C	0.8484	1.0702	-0.2839
C	1.3831	-0.1744	0.0488	C	1.3831	-0.1744	0.0486
C	0.5347	-1.2446	0.3326	C	0.5347	-1.2446	0.3324
C	-0.8483	-1.0701	0.284	C	-0.8483	-1.0701	0.2838
C	-1.383	0.1745	-0.0484	C	-1.383	0.1745	-0.0486
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.2447	-0.3325
C	1.0525	-2.4502	0.6546	C	1.0525	-2.4502	0.6544
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.4502	-0.6545
N	-0.2198	3.5006	-0.933	N	-0.3674	3.5943	-0.3448
O	-0.7243	4.6749	-1.2466	O	-0.8719	4.7686	-0.6584
N	0.2198	-3.5005	0.9331	N	0.3674	-3.5943	0.3447
O	0.7243	-4.6749	1.2467	O	0.8719	-4.7686	0.6583
O	-2.2503	2.6014	-0.6964	O	-2.1201	2.5187	-1.2157
O	2.2503	-2.6013	0.6967	O	2.1201	-2.5186	1.2157
Br	-1.9924	-2.5133	0.6668	Br	-1.9924	-2.5133	0.6666
H	1.5174	1.9142	-0.5076	H	1.5174	1.9142	-0.5078

H	2.4737	-0.312	0.0872	H	2.4737	-0.312	0.087
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.3121	-0.0868
H	0.7836	3.374	-0.8977	H	0.5269	3.537	0.1253
H	-0.1513	5.3976	-1.4384	H	-0.4004	5.5558	-0.4454
H	-0.7836	-3.3739	0.8978	H	-0.5269	-3.5369	-0.1255
H	0.1513	-5.3976	1.4384	H	0.4005	-5.5558	0.4452
	60°				**90°**		
C	0.8484	1.0702	-0.2839	C	0.8484	1.0702	-0.2839
C	1.3831	-0.1744	0.0486	C	1.3831	-0.1744	0.0486
C	0.5347	-1.2446	0.3324	C	0.5347	-1.2446	0.3324
C	-0.8483	-1.0701	0.2838	C	-0.8483	-1.0701	0.2838
C	-1.383	0.1745	-0.0486	C	-1.383	0.1745	-0.0486
C	-0.5346	1.2447	-0.3325	C	-0.5346	1.2447	-0.3325
C	1.0525	-2.4502	0.6544	C	1.0525	-2.4502	0.6544
C	-1.0525	2.4502	-0.6545	C	-1.0525	2.4502	-0.6545
N	-0.7688	3.5452	0.1168	N	-1.3166	3.3663	0.3281
O	-1.2733	4.7194	-0.1968	O	-1.8211	4.5406	0.0144
N	0.7689	-3.5451	-0.1169	N	1.3166	-3.3662	-0.328
O	1.2734	-4.7195	0.1968	O	1.8211	-4.5406	-0.0143
O	-1.7659	2.562	-1.623	O	-1.2826	2.7199	-1.8093
O	1.7658	-2.562	1.623	O	1.2824	-2.7198	1.8093
Br	-1.9924	-2.5133	0.6666	Br	-1.9924	-2.5133	0.6666
H	1.5174	1.9142	-0.5078	H	1.5174	1.9142	-0.5078
H	2.4737	-0.312	0.087	H	2.4737	-0.312	0.087
H	-2.4737	0.3121	-0.0868	H	-2.4737	0.3121	-0.0868
H	-0.1712	3.4515	0.9281	H	-1.1239	3.1404	1.2955
H	-1.0781	5.4729	0.3339	H	-2.0028	5.1709	0.6905
H	0.1714	-3.4514	-0.9282	H	1.1241	-3.1403	-1.2955
H	1.0782	-5.4729	-0.3339	H	2.0028	-5.1709	-0.6903
	120°				**150°**		
C	0.8484	1.0703	-0.2839	C	0.8485	1.0703	-0.2838
C	1.3831	-0.1743	0.0486	C	1.3832	-0.1743	0.0487
C	0.5347	-1.2445	0.3324	C	0.5348	-1.2445	0.3325
C	-0.8483	-1.07	0.2838	C	-0.8482	-1.07	0.2839
C	-1.383	0.1746	-0.0486	C	-1.3829	0.1746	-0.0485
C	-0.5346	1.2448	-0.3325	C	-0.5345	1.2448	-0.3324
C	1.0525	-2.4501	0.6544	C	1.0526	-2.4501	0.6545
C	-1.0525	2.4503	-0.6545	C	-1.0524	2.4503	-0.6544
N	-1.8639	3.1057	0.2324	N	-2.264	2.8331	-0.1447
O	-2.3684	4.2799	-0.0813	O	-2.7685	4.0073	-0.4584
N	1.864	-3.1055	-0.2322	N	2.2642	-2.8328	0.1449
O	2.3684	-4.2799	0.0816	O	2.7685	-4.0072	0.4587
O	-0.7996	2.95	-1.7248	O	-0.4465	3.1907	-1.3921
O	0.7995	-2.9497	1.7248	O	0.4464	-3.1902	1.3921
Br	-1.9924	-2.5132	0.6666	Br	-1.9923	-2.5132	0.6667

H	1.5174	1.9143	-0.5078	H	1.5175	1.9143	-0.5077
H	2.4737	-0.3119	0.087	H	2.4738	-0.3119	0.0871
H	-2.4737	0.3122	-0.0868	H	-2.4736	0.3122	-0.0867
H	-2.0757	2.687	1.129	H	-2.7717	2.2129	0.4733
H	-2.9267	4.7309	0.5289	H	-3.6022	4.2707	-0.1075
H	2.0759	-2.6869	-1.1289	H	2.772	-2.2128	-0.473
H	2.9267	-4.7309	-0.5286	H	3.6022	-4.2707	0.108
180°				**210°**			
C	0.8486	1.0704	-0.284	C	0.8486	1.0704	-0.2839
C	1.3833	-0.1742	0.0485	C	1.3833	-0.1742	0.0486
C	0.5349	-1.2444	0.3323	C	0.5349	-1.2444	0.3324
C	-0.8481	-1.0699	0.2837	C	-0.8481	-1.0699	0.2838
C	-1.3828	0.1747	-0.0487	C	-1.3828	0.1747	-0.0486
C	-0.5344	1.2449	-0.3326	C	-0.5344	1.2449	-0.3325
C	1.0527	-2.45	0.6543	C	1.0527	-2.45	0.6544
C	-1.0523	2.4504	-0.6546	C	-1.0523	2.4504	-0.6545
N	-2.4098	2.6216	-0.7022	N	-2.2622	2.5279	-1.2905
O	-2.9143	3.7959	-1.0159	O	-2.7667	3.7022	-1.6042
N	2.41	-2.6213	0.7021	N	2.2625	-2.5275	1.2904
O	2.9144	-3.7957	1.0158	O	2.7668	-3.702	1.6041
O	-0.3177	3.3774	-0.9005	O	-0.4479	3.4601	-0.3813
O	0.3178	-3.3768	0.9001	O	0.4481	-3.4594	0.381
Br	-1.9922	-2.5131	0.6665	Br	-1.9922	-2.5131	0.6666
H	1.5176	1.9144	-0.5079	H	1.5176	1.9144	-0.5078
H	2.4739	-0.3118	0.0869	H	2.4739	-0.3118	0.087
H	-2.4735	0.3123	-0.0869	H	-2.4735	0.3123	-0.0868
H	-3.0253	1.8451	-0.4963	H	-2.7686	1.6821	-1.5194
H	-3.8484	3.9136	-1.0486	H	-3.5993	3.7554	-2.0417
H	3.0256	-1.8449	0.4962	H	2.7689	-1.6819	1.5194
H	3.8484	-3.9136	1.0486	H	3.5993	-3.7554	2.0417
240°				**270°**			
C	0.8486	1.0704	-0.2838	C	0.8484	1.0704	-0.2837
C	1.3833	-0.1742	0.0487	C	1.3831	-0.1742	0.0488
C	0.5349	-1.2444	0.3325	C	0.5347	-1.2444	0.3326
C	-0.8481	-1.0699	0.2839	C	-0.8483	-1.0699	0.284
C	-1.3828	0.1747	-0.0485	C	-1.383	0.1747	-0.0484
C	-0.5344	1.2449	-0.3324	C	-0.5346	1.2449	-0.3323
C	1.0527	-2.45	0.6545	C	1.0525	-2.45	0.6546
C	-1.0523	2.4504	-0.6544	C	-1.0525	2.4504	-0.6543
N	-1.8608	2.577	-1.752	N	-1.3132	2.7559	-1.9632
O	-2.3652	3.7513	-2.0657	O	-1.8177	3.9302	-2.2769
N	1.861	-2.5767	1.752	N	1.313	-2.7556	1.9633
O	2.3653	-3.7512	2.0657	O	1.8174	-3.9301	2.2769
O	-0.8021	3.4167	0.0261	O	-1.2856	3.2588	0.2125
O	0.8024	-3.4161	-0.0262	O	1.2855	-3.2583	-0.2125

Br	-1.9922	-2.5131	0.6667	Br	-1.9924	-2.5131	0.6668
H	1.5176	1.9144	-0.5077	H	1.5174	1.9144	-0.5076
H	2.4739	-0.3118	0.0871	H	2.4737	-0.3118	0.0872
H	-2.4735	0.3123	-0.0867	H	-2.4737	0.3123	-0.0866
H	-2.0704	1.7676	-2.3221	H	-1.1179	2.0787	-2.6894
H	-2.9216	3.8384	-2.8209	H	-1.9971	4.1403	-3.1774
H	2.0707	-1.7674	2.3222	H	1.1178	-2.0785	2.6896
H	2.9216	-3.8384	2.8209	H	1.9967	-4.1403	3.1774
300°				**330°**			
C	0.8484	1.0704	-0.2837	C	0.8484	1.0703	-0.2837
C	1.3831	-0.1742	0.0488	C	1.3831	-0.1743	0.0488
C	0.5347	-1.2444	0.3326	C	0.5347	-1.2445	0.3326
C	-0.8483	-1.0699	0.284	C	-0.8483	-1.07	0.284
C	-1.383	0.1747	-0.0484	C	-1.383	0.1746	-0.0484
C	-0.5346	1.2449	-0.3323	C	-0.5346	1.2448	-0.3323
C	1.0525	-2.45	0.6546	C	1.0525	-2.4501	0.6546
C	-1.0525	2.4504	-0.6543	C	-1.0525	2.4503	-0.6543
N	-1.3132	2.7559	-1.9632	N	-0.3657	3.2891	-1.4903
O	-1.8177	3.9302	-2.2769	O	-0.8702	4.4634	-1.8039
N	1.313	-2.7556	1.9633	N	0.3656	-3.289	1.4905
O	1.8174	-3.9301	2.2769	O	0.8701	-4.4634	1.804
O	-1.2856	3.2588	0.2125	O	-2.1216	2.7881	-0.2046
O	1.2855	-3.2583	-0.2125	O	2.1216	-2.7879	0.2049
Br	-1.9924	-2.5131	0.6668	Br	-1.9924	-2.5132	0.6668
H	1.5174	1.9144	-0.5076	H	1.5174	1.9143	-0.5076
H	2.4737	-0.3118	0.0872	H	2.4737	-0.3119	0.0872
H	-2.4737	0.3123	-0.0866	H	-2.4737	0.3122	-0.0866
H	-1.1179	2.0787	-2.6894	H	0.5299	3.0062	-1.867
H	-1.9971	4.1403	-3.1774	H	-0.3976	5.0405	-2.3793
H	1.1178	-2.0785	2.6896	H	-0.53	-3.006	1.8672
H	1.9967	-4.1403	3.1774	H	0.3974	-5.0405	2.3793

Table S15 Cartesian coordinates of the H_2-BrH-BDHA ligand geometry after counter-rotation of both hydroxamate groups.

0°				**30°**			
C	0.8484	1.0702	-0.2837	C	0.8484	1.3279	0.298
C	1.3831	-0.1744	0.0488	C	1.3831	0.0833	0.6305
C	0.5347	-1.2446	0.3326	C	0.5347	-0.9869	0.9143
C	-0.8483	-1.0701	0.284	C	-0.8483	-0.8124	0.8657
C	-1.383	0.1745	-0.0484	C	-1.383	0.4322	0.5333
C	-0.5346	1.2447	-0.3323	C	-0.5346	1.5024	0.2494
C	1.0525	-2.4502	0.6546	C	1.0525	-2.1925	1.2363
C	-1.0525	2.4502	-0.6543	C	-1.0525	2.7079	-0.0726
N	-0.2198	3.5006	-0.933	N	-0.3657	3.5467	-0.9086

O	-0.7243	4.6749	-1.2466	O	-0.8701	4.721	-1.2222
N	0.2198	-3.5005	0.9331	N	0.3674	-3.3366	0.9266
O	0.7243	-4.6749	1.2467	O	0.8719	-4.5109	1.2402
O	-2.2503	2.6014	-0.6964	O	-2.1216	3.0457	0.3771
O	2.2503	-2.6013	0.6967	O	2.1201	-2.2609	1.7976
Br	-1.9924	-2.5133	0.6668	Br	-1.9924	-2.2556	1.2485
H	1.5174	1.9142	-0.5076	H	1.5174	2.1719	0.0741
H	2.4737	-0.312	0.0872	H	2.4737	-0.0543	0.6689
H	-2.4737	0.3121	-0.0866	H	-2.4737	0.5698	0.4951
H	0.7836	3.374	-0.8977	H	0.5299	3.2638	-1.2853
H	-0.1513	5.3976	-1.4384	H	-0.3976	5.2981	-1.7976
H	-0.7836	-3.3739	0.8978	H	-0.5269	-3.2792	0.4564
H	0.1513	-5.3976	1.4384	H	0.4005	-5.2981	1.0271
	60°				**90°**		
C	0.8484	1.5165	0.4126	C	0.8484	1.5856	0.4003
C	1.3831	0.2719	0.7451	C	1.3831	0.341	0.7328
C	0.5347	-0.7983	1.0289	C	0.5347	-0.7292	1.0166
C	-0.8483	-0.6238	0.9803	C	-0.8483	-0.5547	0.968
C	-1.383	0.6208	0.6479	C	-1.383	0.6899	0.6356
C	-0.5346	1.691	0.364	C	-0.5346	1.7601	0.3517
C	1.0525	-2.0039	1.3509	C	1.0525	-1.9348	1.3386
C	-1.0525	2.8965	0.042	C	-1.0525	2.9656	0.0297
N	-0.7659	3.4627	-1.1711	N	-1.3132	3.2711	-1.2792
O	-1.2704	4.637	-1.4847	O	-1.8177	4.4454	-1.5929
N	0.7689	-3.0988	0.5796	N	1.3166	-2.8508	0.3561
O	1.2734	-4.2731	0.8933	O	1.8211	-4.0252	0.6698
O	-1.7685	3.4749	0.8244	O	-1.2856	3.774	0.8965
O	1.7658	-2.1157	2.3195	O	1.2824	-2.2044	2.4935
Br	-1.9924	-2.067	1.3631	Br	-1.9924	-1.9979	1.3508
H	1.5174	2.3605	0.1887	H	1.5174	2.4296	0.1764
H	2.4737	0.1343	0.7835	H	2.4737	0.2034	0.7712
H	-2.4737	0.7584	0.6097	H	-2.4737	0.8275	0.5974
H	-0.1661	2.9782	-1.8265	H	-1.1179	2.5939	-2.0054
H	-1.0732	5.0265	-2.3195	H	-1.9971	4.6555	-2.4935
H	0.1714	-3.0051	-0.2317	H	1.1241	-2.6249	-0.6114
H	1.0782	-5.0265	0.3626	H	2.0028	-4.6555	-0.0062
	120°				**150°**		
C	0.846	1.5166	0.2642	C	0.8471	1.328	0.0409
C	1.3807	0.272	0.5967	C	1.3818	0.0834	0.3734
C	0.5323	-0.7982	0.8805	C	0.5334	-0.9868	0.6572
C	-0.8507	-0.6237	0.8319	C	-0.8496	-0.8123	0.6086
C	-1.3854	0.6209	0.4995	C	-1.3843	0.4323	0.2762
C	-0.537	1.6911	0.2156	C	-0.5359	1.5025	-0.0077
C	1.0501	-2.0038	1.2025	C	1.0512	-2.1924	0.9792
C	-1.0549	2.8966	-0.1064	C	-1.0538	2.708	-0.3297

N	-1.8634	3.0232	-1.204	N	-2.2638	2.7855	-0.9656
O	-2.3679	4.1975	-1.5177	O	-2.7682	3.9598	-1.2793
N	1.8615	-2.6592	0.3158	N	2.2628	-2.5751	0.4696
O	2.3659	-3.8335	0.6296	O	2.7671	-3.7496	0.7834
O	-0.8047	3.8629	0.5741	O	-0.4494	3.7177	-0.0565
O	0.797	-2.5034	2.2729	O	0.445	-2.9325	1.7168
Br	-1.9948	-2.0669	1.2147	Br	-1.9937	-2.2555	0.9914
H	1.515	2.3606	0.0403	H	1.5161	2.172	-0.183
H	2.4713	0.1344	0.6351	H	2.4724	-0.0542	0.4118
H	-2.4761	0.7585	0.4613	H	-2.475	0.5699	0.238
H	-2.073	2.2138	-1.7741	H	-2.7701	1.9397	-1.1945
H	-2.9242	4.2845	-2.2729	H	-3.6008	4.013	-1.7168
H	2.0735	-2.2406	-0.5808	H	2.7705	-1.9551	-0.1482
H	2.9242	-4.2845	0.0195	H	3.6008	-4.013	0.4327
180°				**210°**			
C	0.8486	1.0704	-0.284	C	0.85	0.8127	-0.6087
C	1.3833	-0.1742	0.0485	C	1.3847	-0.4318	-0.2762
C	0.5349	-1.2444	0.3323	C	0.5363	-1.502	0.0076
C	-0.8481	-1.0699	0.2837	C	-0.8467	-1.3275	-0.041
C	-1.3828	0.1747	-0.0487	C	-1.3814	-0.083	-0.3734
C	-0.5344	1.2449	-0.3326	C	-0.533	0.9872	-0.6573
C	1.0527	-2.45	0.6543	C	1.0541	-2.7076	0.3296
C	-1.0523	2.4504	-0.6546	C	-1.0509	2.1927	-0.9793
N	-2.4098	2.6216	-0.7022	N	-2.2625	2.5755	-0.4695
O	-2.9143	3.7959	-1.0159	O	-2.767	3.7497	-0.7832
N	2.41	-2.6213	0.7021	N	2.2639	-2.7852	0.9656
O	2.9144	-3.7957	1.0158	O	2.7682	-3.9597	1.2793
O	-0.3177	3.3774	-0.9005	O	-0.4449	2.9331	-1.7169
O	0.3178	-3.3768	0.9001	O	0.4495	-3.7171	0.0563
Br	-1.9922	-2.5131	0.6665	Br	-1.9908	-2.7707	0.3418
H	1.5176	1.9144	-0.5079	H	1.519	1.6567	-0.8326
H	2.4739	-0.3118	0.0869	H	2.4753	-0.5694	-0.2378
H	-2.4735	0.3123	-0.0869	H	-2.4721	0.0546	-0.4116
H	-3.0253	1.8451	-0.4963	H	-2.7701	1.9553	0.1484
H	-3.8484	3.9136	-1.0486	H	-3.6007	4.0131	-0.4324
H	3.0256	-1.8449	0.4962	H	2.7704	-1.9396	1.1946
H	3.8484	-3.9136	1.0486	H	3.6007	-4.0131	1.7169
240°				**270°**			
C	0.8511	0.6241	-0.8319	C	0.8484	0.555	-0.9679
C	1.3858	-0.6205	-0.4994	C	1.3831	-0.6896	-0.6354
C	0.5374	-1.6907	-0.2156	C	0.5347	-1.7598	-0.3516
C	-0.8456	-1.5162	-0.2642	C	-0.8483	-1.5853	-0.4002
C	-1.3803	-0.2716	-0.5966	C	-1.383	-0.3407	-0.7326
C	-0.5319	0.7986	-0.8805	C	-0.5346	0.7295	-1.0165
C	1.0552	-2.8963	0.1064	C	1.0525	-2.9654	-0.0296

C	-1.0498	2.0041	-1.2025	C	-1.0525	1.935	-1.3385
N	-1.8612	2.6595	-0.3156	N	-1.3166	2.8511	-0.3559
O	-2.3658	3.8338	-0.6293	O	-1.8211	4.0254	-0.6696
N	1.8635	-3.023	1.204	N	1.313	-3.271	1.2792
O	2.3678	-4.1975	1.5176	O	1.8174	-4.4455	1.5928
O	-0.797	2.5039	-2.2729	O	-1.2826	2.2047	-2.4933
O	0.8048	-3.8624	-0.5742	O	1.2855	-3.7737	-0.8966
Br	-1.9897	-2.9594	0.1186	Br	-1.9924	-3.0285	-0.0174
H	1.5201	1.4681	-1.0558	H	1.5174	1.399	-1.1918
H	2.4764	-0.7581	-0.461	H	2.4737	-0.8272	-0.597
H	-2.471	-0.134	-0.6348	H	-2.4737	-0.2031	-0.7708
H	-2.0731	2.2409	0.581	H	-1.1239	2.6252	0.6115
H	-2.924	4.2847	-0.0191	H	-2.0028	4.6557	0.0065
H	2.0731	-2.2137	1.7742	H	1.1178	-2.5939	2.0055
H	2.924	-4.2847	2.2729	H	1.9967	-4.6557	2.4933
300°				**330°**			
C	0.8484	0.624	-0.9802	C	0.8484	0.8126	-0.8656
C	1.3831	-0.6206	-0.6477	C	1.3831	-0.432	-0.5331
C	0.5347	-1.6908	-0.3639	C	0.5347	-1.5022	-0.2493
C	-0.8483	-1.5163	-0.4125	C	-0.8483	-1.3277	-0.2979
C	-1.383	-0.2717	-0.7449	C	-1.383	-0.0831	-0.6303
C	-0.5346	0.7985	-1.0288	C	-0.5346	0.9871	-0.9142
C	1.0525	-2.8964	-0.0419	C	1.0525	-2.7078	0.0727
C	-1.0525	2.004	-1.3508	C	-1.0525	2.1926	-1.2362
N	-0.7688	3.099	-0.5795	N	-0.3674	3.3367	-0.9265
O	-1.2733	4.2733	-0.8931	O	-0.8719	4.511	-1.2401
N	0.7658	-3.4626	1.171	N	0.3656	-3.5466	0.9086
O	1.2702	-4.6371	1.4846	O	0.8701	-4.7211	1.2221
O	-1.7659	2.1159	-2.3193	O	-2.1201	2.2611	-1.7974
O	1.7685	-3.4747	-0.8244	O	2.1216	-3.0456	-0.377
Br	-1.9924	-2.9595	-0.0297	Br	-1.9924	-2.7709	0.0849
H	1.5174	1.468	-1.2041	H	1.5174	1.6566	-1.0895
H	2.4737	-0.7582	-0.6093	H	2.4737	-0.5696	-0.4947
H	-2.4737	-0.1341	-0.7831	H	-2.4737	0.0545	-0.6685
H	-0.1712	3.0053	0.2318	H	0.5269	3.2794	-0.4564
H	-1.0781	5.0267	-0.3624	H	-0.4004	5.2982	-1.0271
H	0.1659	-2.9782	1.8265	H	-0.53	-3.2637	1.2853
H	1.0729	-5.0267	2.3193	H	0.3974	-5.2982	1.7974

Table S16 Cartesian coordinates of the rotated geometry for the hydroxamate group distal to the F side in the PDDH ligand.

0°				**30°**			
C	1.1421	0.7402	-0.1063	C	1.1421	0.7766	0.3402
C	1.2382	-0.6462	-0.0457	C	1.2382	-0.6098	0.4008

C	0.0676	-1.3806	0.0578	C	0.0676	-1.3442	0.5043
N	-1.1644	-0.8283	0.1035	N	-1.1644	-0.7919	0.55
C	-1.226	0.5198	0.0427	C	-1.226	0.5562	0.4892
C	-0.1128	1.3385	-0.0615	C	-0.1128	1.3749	0.385
C	0.164	-2.7269	0.1164	C	0.164	-2.6905	0.5629
C	-0.243	2.682	-0.118	C	-0.243	2.7184	0.3285
N	0.8692	3.4737	-0.2209	N	0.6767	3.467	-0.3557
O	0.7424	4.7824	-0.276	O	0.5499	4.7757	-0.4108
N	-0.9677	-3.4904	0.2191	N	-0.9677	-3.454	0.6656
O	-0.8737	-4.8018	0.2761	O	-0.8737	-4.7654	0.7226
O	-1.3406	3.1847	-0.0778	O	-1.1708	3.2591	0.8814
O	1.2488	-3.257	0.0783	O	1.2488	-3.2206	0.5248
H	2.0491	1.357	-0.1887	H	2.0491	1.3934	0.2578
H	2.2173	-1.1463	-0.079	H	2.2173	-1.1099	0.3675
H	-2.2173	0.9952	0.078	H	-2.2173	1.0316	0.5245
H	1.7887	3.0525	-0.2545	H	1.4541	3.0139	-0.8188
H	1.5077	5.3272	-0.3467	H	1.1828	5.2908	-0.8814
H	-1.8765	-3.0463	0.251	H	-1.8765	-3.0099	0.6975
H	-1.6524	-5.3272	0.3467	H	-1.6524	-5.2908	0.7932
	60°				**90°**		
C	1.1421	0.8283	0.5036	C	1.1421	0.8816	0.5524
C	1.2382	-0.5581	0.5642	C	1.2382	-0.5048	0.613
C	0.0676	-1.2925	0.6677	C	0.0676	-1.2392	0.7165
N	-1.1644	-0.7402	0.7134	N	-1.1644	-0.6869	0.7622
C	-1.226	0.6079	0.6526	C	-1.226	0.6612	0.7014
C	-0.1128	1.4266	0.5484	C	-0.1128	1.4799	0.5972
C	0.164	-2.6388	0.7263	C	0.164	-2.5855	0.7751
C	-0.243	2.7701	0.4919	C	-0.243	2.8234	0.5407
N	0.2202	3.4574	-0.5978	N	-0.3782	3.4476	-0.6702
O	0.0933	4.7661	-0.6529	O	-0.5051	4.7563	-0.7253
N	-0.9677	-3.4023	0.829	N	-0.9677	-3.349	0.8778
O	-0.8737	-4.7137	0.886	O	-0.8737	-4.6604	0.9348
O	-0.7681	3.3649	1.4027	O	-0.2402	3.4738	1.5586
O	1.2488	-3.1689	0.6882	O	1.2488	-3.1156	0.737
H	2.0491	1.4451	0.4212	H	2.0491	1.4984	0.47
H	2.2173	-1.0582	0.5309	H	2.2173	-1.0049	0.5797
H	-2.2173	1.0833	0.6879	H	-2.2173	1.1366	0.7367
H	0.6601	2.9591	-1.3608	H	-0.3804	2.9026	-1.5229
H	0.4121	5.2391	-1.4027	H	-0.598	5.1858	-1.5586
H	-1.8765	-2.9582	0.8609	H	-1.8765	-2.9049	0.9097
H	-1.6524	-5.2391	0.9566	H	-1.6524	-5.1858	1.0054
	120°				**150°**		
C	1.1421	0.9221	0.4736	C	1.1645	0.9389	0.2757
C	1.2382	-0.4643	0.5342	C	1.2606	-0.4475	0.3363
C	0.0676	-1.1987	0.6377	C	0.09	-1.1819	0.4398

N	-1.1644	-0.6464	0.6834	N	-1.142	-0.6296	0.4855
C	-1.226	0.7017	0.6226	C	-1.2036	0.7185	0.4247
C	-0.1128	1.5204	0.5184	C	-0.0904	1.5372	0.3205
C	0.164	-2.545	0.6963	C	0.1864	-2.5282	0.4984
C	-0.243	2.8639	0.4619	C	-0.2206	2.8807	0.264
N	-0.958	3.4401	-0.5535	N	-1.3415	3.437	-0.2914
O	-1.0849	4.7488	-0.6085	O	-1.4684	4.7457	-0.3464
N	-0.9677	-3.3085	0.799	N	-0.9453	-3.2917	0.6011
O	-0.8737	-4.6199	0.856	O	-0.8513	-4.6031	0.6581
O	0.2713	3.5566	1.3073	O	0.6518	3.5911	0.7036
O	1.2488	-3.0751	0.6582	O	1.2712	-3.0583	0.4603
H	2.0491	1.5389	0.3912	H	2.0715	1.5557	0.1933
H	2.2173	-0.9644	0.5009	H	2.2397	-0.9476	0.303
H	-2.2173	1.1771	0.6579	H	-2.1949	1.1939	0.46
H	-1.3888	2.8597	-1.2617	H	-2.0724	2.8418	-0.6597
H	-1.5768	5.1453	-1.3073	H	-2.2397	5.1285	-0.7287
H	-1.8765	-2.8644	0.8309	H	-1.8541	-2.8476	0.633
H	-1.6524	-5.1453	0.9266	H	-1.63	-5.1285	0.7287
180°				**210°**			
C	1.2685	0.9277	-0.1753	C	1.1421	0.8913	-0.2527
C	1.3646	-0.4587	-0.1147	C	1.2382	-0.4951	-0.1921
C	0.194	-1.1931	-0.0112	C	0.0676	-1.2295	-0.0886
N	-1.038	-0.6408	0.0345	N	-1.1644	-0.6772	-0.0429
C	-1.0996	0.7073	-0.0263	C	-1.226	0.6709	-0.1037
C	0.0136	1.526	-0.1305	C	-0.1128	1.4896	-0.2079
C	0.2904	-2.5394	0.0474	C	0.164	-2.5758	-0.03
C	-0.1166	2.8695	-0.187	C	-0.243	2.8331	-0.2644
N	-1.3607	3.4391	-0.1413	N	-1.2947	3.4458	0.3624
O	-1.4876	4.7478	-0.1963	O	-1.4215	4.7545	0.3075
N	-0.8413	-3.3029	0.1501	N	-0.9677	-3.3393	0.0727
O	-0.7473	-4.6143	0.2071	O	-0.8737	-4.6507	0.1297
O	0.8646	3.5681	-0.2777	O	0.5684	3.4937	-0.8679
O	1.3752	-3.0695	0.0093	O	1.2488	-3.1059	-0.0681
H	2.1755	1.5445	-0.2577	H	2.0491	1.5081	-0.3351
H	2.3437	-0.9588	-0.148	H	2.2173	-0.9952	-0.2254
H	-2.0909	1.1827	0.009	H	-2.2173	1.1463	-0.0684
H	-2.1827	2.8537	-0.0654	H	-1.9745	2.8923	0.8679
H	-2.3437	5.1397	-0.165	H	-2.1452	5.1761	0.7387
H	-1.7501	-2.8588	0.182	H	-1.8765	-2.8952	0.1046
H	-1.526	-5.1397	0.2777	H	-1.6524	-5.1761	0.2003
240°				**270°**			
C	1.1421	0.8396	-0.4265	C	1.1421	0.7863	-0.4785
C	1.2382	-0.5468	-0.3659	C	1.2382	-0.6001	-0.4179
C	0.0676	-1.2812	-0.2624	C	0.0676	-1.3345	-0.3144
N	-1.1644	-0.7289	-0.2167	N	-1.1644	-0.7822	-0.2687

C	-1.226	0.6192	-0.2775	C	-1.226	0.5659	-0.3295
C	-0.1128	1.4379	-0.3817	C	-0.1128	1.3846	-0.4337
C	0.164	-2.6275	-0.2038	C	0.164	-2.6808	-0.2558
C	-0.243	2.7814	-0.4382	C	-0.243	2.7281	-0.4902
N	-0.8381	3.4553	0.5942	N	-0.2397	3.4652	0.6635
O	-0.9649	4.7641	0.5393	O	-0.3665	4.7739	0.6085
N	-0.9677	-3.391	-0.1011	N	-0.9677	-3.4443	-0.1531
O	-0.8737	-4.7024	-0.0441	O	-0.8737	-4.7557	-0.0961
O	0.1657	3.3879	-1.3995	O	-0.3622	3.279	-1.5585
O	1.2488	-3.1576	-0.2419	O	1.2488	-3.2109	-0.2939
H	2.0491	1.4564	-0.5089	H	2.0491	1.4031	-0.5609
H	2.2173	-1.0469	-0.3992	H	2.2173	-1.1002	-0.4512
H	-2.2173	1.0946	-0.2422	H	-2.2173	1.0413	-0.2942
H	-1.1805	2.9471	1.3995	H	-0.1399	3.0036	1.5585
H	-1.3745	5.2278	1.2496	H	-0.3644	5.2811	1.4024
H	-1.8765	-2.9469	-0.0692	H	-1.8765	-3.0002	-0.1212
H	-1.6524	-5.2278	0.0265	H	-1.6524	-5.2811	-0.0255
300°				**330°**			
C	1.1421	0.7458	-0.3947	C	1.1421	0.7289	-0.1977
C	1.2382	-0.6406	-0.3341	C	1.2382	-0.6575	-0.1371
C	0.0676	-1.375	-0.2306	C	0.0676	-1.3919	-0.0336
N	-1.1644	-0.8227	-0.1849	N	-1.1644	-0.8396	0.0121
C	-1.226	0.5254	-0.2457	C	-1.226	0.5085	-0.0487
C	-0.1128	1.3441	-0.3499	C	-0.1128	1.3272	-0.1529
C	0.164	-2.7213	-0.172	C	0.164	-2.7382	0.025
C	-0.243	2.6876	-0.4064	C	-0.243	2.6707	-0.2094
N	0.3401	3.4727	0.5518	N	0.746	3.4758	0.2888
O	0.2133	4.7814	0.4967	O	0.6192	4.7845	0.2338
N	-0.9677	-3.4848	-0.0693	N	-0.9677	-3.5017	0.1277
O	-0.8737	-4.7962	-0.0123	O	-0.8737	-4.8131	0.1847
O	-0.8737	3.1962	-1.3023	O	-1.2318	3.1617	-0.6995
O	1.2488	-3.2514	-0.2101	O	1.2488	-3.2683	-0.0131
H	2.0491	1.3626	-0.4771	H	2.0491	1.3457	-0.2801
H	2.2173	-1.1407	-0.3674	H	2.2173	-1.1576	-0.1704
H	-2.2173	1.0008	-0.2104	H	-2.2173	0.9839	-0.0134
H	0.8684	3.0465	1.3023	H	1.5743	3.0644	0.6995
H	0.6144	5.3216	1.1561	H	1.2996	5.3385	0.5767
H	-1.8765	-3.0407	-0.0374	H	-1.8765	-3.0576	0.1596
H	-1.6524	-5.3216	0.0583	H	-1.6524	-5.3385	0.2553

Table S17 Cartesian coordinates of the rotated geometry for the hydroxamate group proximal to the F side in the PDDH ligand.

0°				**30°**			
C	1.1421	0.7402	-0.1063	C	1.1421	0.7548	-0.0135

C	1.2382	-0.6462	-0.0457	C	1.2382	-0.6316	0.0471
C	0.0676	-1.3806	0.0578	C	0.0676	-1.366	0.1506
N	-1.1644	-0.8283	0.1035	N	-1.1644	-0.8137	0.1963
C	-1.226	0.5198	0.0427	C	-1.226	0.5344	0.1355
C	-0.1128	1.3385	-0.0615	C	-0.1128	1.3531	0.0313
C	0.164	-2.7269	0.1164	C	0.164	-2.7123	0.2092
C	-0.243	2.682	-0.118	C	-0.243	2.6966	-0.0252
N	0.8692	3.4737	-0.2209	N	0.8692	3.4883	-0.1281
O	0.7424	4.7824	-0.276	O	0.7424	4.797	-0.1832
N	-0.9677	-3.4904	0.2191	N	-0.8441	-3.4931	-0.2891
O	-0.8737	-4.8018	0.2761	O	-0.7501	-4.8045	-0.232
O	-1.3406	3.1847	-0.0778	O	-1.3406	3.1993	0.0149
O	1.2488	-3.257	0.0783	O	1.1398	-3.2271	0.7013
H	2.0491	1.357	-0.1887	H	2.0491	1.3716	-0.096
H	2.2173	-1.1463	-0.079	H	2.2173	-1.1317	0.0138
H	-2.2173	0.9952	0.078	H	-2.2173	1.0098	0.1708
H	1.7887	3.0525	-0.2545	H	1.7887	3.0671	-0.1617
H	1.5077	5.3272	-0.3467	H	1.5077	5.3418	-0.254
H	-1.8765	-3.0463	0.251	H	-1.6615	-3.0618	-0.7013
H	-1.6524	-5.3272	0.3467	H	-1.4438	-5.3418	-0.5748
	60°				**90°**		
C	1.1421	0.7471	0.1833	C	1.1421	0.7191	0.2668
C	1.2382	-0.6393	0.2439	C	1.2382	-0.6673	0.3274
C	0.0676	-1.3737	0.3474	C	0.0676	-1.4017	0.4309
N	-1.1644	-0.8214	0.3931	N	-1.1644	-0.8494	0.4766
C	-1.226	0.5267	0.3323	C	-1.226	0.4987	0.4158
C	-0.1128	1.3454	0.2281	C	-0.1128	1.3174	0.3116
C	0.164	-2.72	0.406	C	0.164	-2.748	0.4895
C	-0.243	2.6889	0.1716	C	-0.243	2.6609	0.2551
N	0.8692	3.4806	0.0687	N	0.8692	3.4526	0.1522
O	0.7424	4.7893	0.0136	O	0.7424	4.7613	0.0971
N	-0.4373	-3.4917	-0.5517	N	0.1437	-3.4865	-0.663
O	-0.3433	-4.8031	-0.4946	O	0.2377	-4.7979	-0.6059
O	-1.3406	3.1916	0.2117	O	-1.3406	3.1637	0.2952
O	0.7808	-3.2429	1.3035	O	0.2681	-3.3001	1.5589
H	2.0491	1.3639	0.1008	H	2.0491	1.3359	0.1843
H	2.2173	-1.1394	0.2106	H	2.2173	-1.1674	0.2941
H	-2.2173	1.0021	0.3676	H	-2.2173	0.9741	0.4511
H	1.7887	3.0594	0.0351	H	1.7887	3.0314	0.1186
H	1.5077	5.334	-0.0571	H	1.5077	5.3061	0.0263
H	-0.954	-3.0536	-1.3035	H	0.0565	-3.024	-1.5589
H	-0.7571	-5.334	-1.1536	H	0.2237	-5.3061	-1.399
	120°				**150°**		
C	1.1421	0.6784	0.2146	C	1.1421	0.6358	0.0406
C	1.2382	-0.708	0.2752	C	1.2382	-0.7506	0.1012

C	0.0676	-1.4424	0.3787	C	0.0676	-1.485	0.2047
N	-1.1644	-0.8901	0.4244	N	-1.1644	-0.9327	0.2504
C	-1.226	0.458	0.3636	C	-1.226	0.4154	0.1896
C	-0.1128	1.2767	0.2594	C	-0.1128	1.2341	0.0854
C	0.164	-2.7887	0.4373	C	0.164	-2.8313	0.2633
C	-0.243	2.6202	0.2028	C	-0.243	2.5776	0.0289
N	0.8692	3.4119	0.1	N	0.8692	3.3693	-0.074
O	0.7424	4.7206	0.0449	O	0.7424	4.678	-0.1291
N	0.7433	-3.479	-0.5933	N	1.2007	-3.4711	-0.3613
O	0.8372	-4.7904	-0.5363	O	1.2946	-4.7825	-0.3042
O	-1.3406	3.1229	0.243	O	-1.3406	3.0804	0.069
O	-0.2609	-3.3834	1.3991	O	-0.6645	-3.4705	0.8668
H	2.0491	1.2952	0.1321	H	2.0491	1.2526	-0.0419
H	2.2173	-1.2081	0.2418	H	2.2173	-1.2507	0.0679
H	-2.2173	0.9334	0.3988	H	-2.2173	0.8908	0.2249
H	1.7887	2.9907	0.0663	H	1.7887	2.9481	-0.1076
H	1.5077	5.2653	-0.0259	H	1.5077	5.2228	-0.1998
H	1.0992	-2.9808	-1.3991	H	1.8948	-2.9356	-0.8668
H	1.2358	-5.2653	-1.2454	H	2.008	-5.2228	-0.7339
	180°				**210°**		
C	1.0841	0.6028	-0.0364	C	1.1421	0.5882	-0.4903
C	1.1802	-0.7836	0.0242	C	1.2382	-0.7982	-0.4297
C	0.0096	-1.518	0.1277	C	0.0676	-1.5326	-0.3262
N	-1.2224	-0.9657	0.1734	N	-1.1644	-0.9803	-0.2805
C	-1.284	0.3824	0.1126	C	-1.226	0.3678	-0.3413
C	-0.1708	1.2011	0.0084	C	-0.1128	1.1865	-0.4455
C	0.106	-2.8643	0.1863	C	0.164	-2.8789	-0.2676
C	-0.3009	2.5446	-0.0481	C	-0.243	2.53	-0.5021
N	0.8112	3.3363	-0.151	N	0.8692	3.3217	-0.6049
O	0.6844	4.645	-0.2061	O	0.7424	4.6304	-0.66
N	1.3354	-3.465	0.1431	N	1.2698	-3.4623	0.29
O	1.4294	-4.7764	0.2002	O	1.3638	-4.7737	0.3471
O	-1.3986	3.0473	-0.008	O	-1.3406	3.0327	-0.4619
O	-0.8926	-3.538	0.2769	O	-0.7255	-3.5679	-0.7073
H	1.9911	1.2196	-0.1189	H	2.0491	1.205	-0.5728
H	2.1594	-1.2837	-0.0091	H	2.2173	-1.2983	-0.4631
H	-2.2753	0.8578	0.1479	H	-2.2173	0.8432	-0.3061
H	1.7308	2.9151	-0.1846	H	1.7887	2.9005	-0.6386
H	1.4497	5.1898	-0.2769	H	1.5077	5.1752	-0.7308
H	2.172	-2.9006	0.0672	H	2.015	-2.8851	0.6584
H	2.2753	-5.1898	0.1704	H	2.1247	-5.1752	0.7308
	240°				**270°**		
C	1.1421	0.5959	-0.6871	C	1.1421	0.6239	-0.7656
C	1.2382	-0.7905	-0.6265	C	1.2382	-0.7625	-0.705
C	0.0676	-1.5249	-0.523	C	0.0676	-1.4969	-0.6015

N	-1.1644	-0.9726	-0.4773	N	-1.1644	-0.9446	-0.5558
C	-1.226	0.3755	-0.5381	C	-1.226	0.4035	-0.6166
C	-0.1128	1.1942	-0.6423	C	-0.1128	1.2222	-0.7208
C	0.164	-2.8712	-0.4645	C	0.164	-2.8432	-0.543
C	-0.243	2.5377	-0.6989	C	-0.243	2.5657	-0.7774
N	0.8692	3.3294	-0.8018	N	0.8692	3.3574	-0.8803
O	0.7424	4.6381	-0.8569	O	0.7424	4.6661	-0.9354
N	0.863	-3.4637	0.5526	N	0.282	-3.4689	0.669
O	0.957	-4.7751	0.6097	O	0.376	-4.7803	0.726
O	-1.3406	3.0405	-0.6587	O	-1.3406	3.0684	-0.7372
O	-0.3666	-3.5521	-1.3095	O	0.1461	-3.4949	-1.5599
H	2.0491	1.2127	-0.7696	H	2.0491	1.2407	-0.8481
H	2.2173	-1.2906	-0.6599	H	2.2173	-1.2626	-0.7384
H	-2.2173	0.8509	-0.5029	H	-2.2173	0.8789	-0.5814
H	1.7887	2.9082	-0.8354	H	1.7887	2.9362	-0.9139
H	1.5077	5.1829	-0.9276	H	1.5077	5.2109	-1.0061
H	1.3075	-2.8933	1.2606	H	0.297	-2.923	1.5209
H	1.4379	-5.1829	1.3095	H	0.4572	-5.2109	1.5599
300°				**330°**			
C	1.1421	0.6646	-0.7165	C	1.1421	0.7072	-0.553
C	1.2382	-0.7218	-0.6559	C	1.2382	-0.6792	-0.4924
C	0.0676	-1.4562	-0.5524	C	0.0676	-1.4136	-0.3889
N	-1.1644	-0.9039	-0.5067	N	-1.1644	-0.8613	-0.3432
C	-1.226	0.4442	-0.5675	C	-1.226	0.4868	-0.404
C	-0.1128	1.2629	-0.6717	C	-0.1128	1.3055	-0.5082
C	0.164	-2.8025	-0.4938	C	0.164	-2.7599	-0.3303
C	-0.243	2.6064	-0.7283	C	-0.243	2.649	-0.5647
N	0.8692	3.3981	-0.8311	N	0.8692	3.4407	-0.6676
O	0.7424	4.7068	-0.8862	O	0.7424	4.7494	-0.7227
N	-0.3175	-3.4764	0.5962	N	-0.7749	-3.4843	0.3537
O	-0.2236	-4.7878	0.6532	O	-0.681	-4.7957	0.4108
O	-1.3406	3.1092	-0.6881	O	-1.3406	3.1517	-0.5246
O	0.6751	-3.4116	-1.4032	O	1.0788	-3.3245	-0.8814
H	2.0491	1.2814	-0.799	H	2.0491	1.324	-0.6355
H	2.2173	-1.2219	-0.6893	H	2.2173	-1.1793	-0.5257
H	-2.2173	0.9196	-0.5323	H	-2.2173	0.9622	-0.3687
H	1.7887	2.9769	-0.8648	H	1.7887	3.0195	-0.7012
H	1.5077	5.2516	-0.957	H	1.5077	5.2942	-0.7934
H	-0.7457	-2.9662	1.358	H	-1.5413	-3.0113	0.8154
H	-0.5549	-5.2516	1.4032	H	-1.3271	-5.2942	0.8814

Table S18 Cartesian coordinates of the PDDH ligand geometry after co-rotation of both hydroxamate groups.

0°	**30°**

C	1.1421	0.7402	-0.1063	C	1.1421	0.7435	-0.1047
C	1.2382	-0.6462	-0.0457	C	1.2382	-0.6429	-0.0441
C	0.0676	-1.3806	0.0578	C	0.0676	-1.3773	0.0594
N	-1.1644	-0.8283	0.1035	N	-1.1644	-0.825	0.1051
C	-1.226	0.5198	0.0427	C	-1.226	0.5231	0.0443
C	-0.1128	1.3385	-0.0615	C	-0.1128	1.3418	-0.0599
C	0.164	-2.7269	0.1164	C	0.164	-2.7236	0.118
C	-0.243	2.682	-0.118	C	-0.243	2.6853	-0.1164
N	0.8692	3.4737	-0.2209	N	0.746	3.4904	0.3818
O	0.7424	4.7824	-0.276	O	0.6192	4.7991	0.3267
N	-0.9677	-3.4904	0.2191	N	-0.8441	-3.5044	-0.3802
O	-0.8737	-4.8018	0.2761	O	-0.7501	-4.8158	-0.3231
O	-1.3406	3.1847	-0.0778	O	-1.2318	3.1763	-0.6065
O	1.2488	-3.257	0.0783	O	1.1397	-3.2384	0.6101
H	2.0491	1.357	-0.1887	H	2.0491	1.3603	-0.1871
H	2.2173	-1.1463	-0.079	H	2.2173	-1.143	-0.0774
H	-2.2173	0.9952	0.078	H	-2.2173	0.9985	0.0796
H	1.7887	3.0525	-0.2545	H	1.5743	3.079	0.7925
H	1.5077	5.3272	-0.3467	H	1.2996	5.3531	0.6697
H	-1.8765	-3.0463	0.251	H	-1.6616	-3.073	-0.7925
H	-1.6524	-5.3272	0.3467	H	-1.4438	-5.3531	-0.666
	60°				**90°**		
C	1.1421	0.7527	-0.1051	C	1.1421	0.7653	-0.1056
C	1.2382	-0.6337	-0.0445	C	1.2382	-0.6211	-0.045
C	0.0676	-1.3681	0.059	C	0.0676	-1.3555	0.0585
N	-1.1644	-0.8158	0.1047	N	-1.1644	-0.8032	0.1042
C	-1.226	0.5323	0.0439	C	-1.226	0.5449	0.0434
C	-0.1128	1.351	-0.0603	C	-0.1128	1.3636	-0.0608
C	0.164	-2.7144	0.1176	C	0.164	-2.7018	0.1171
C	-0.243	2.6945	-0.1168	C	-0.243	2.7071	-0.1173
N	0.3401	3.4796	0.8414	N	-0.2397	3.4441	1.0364
O	0.2133	4.7883	0.7863	O	-0.3665	4.7528	0.9814
N	-0.4374	-3.4861	-0.84	N	0.1436	-3.4404	-1.0355
O	-0.3434	-4.7975	-0.7829	O	0.2376	-4.7518	-0.9783
O	-0.8737	3.2031	-1.0127	O	-0.3622	3.2579	-1.1857
O	0.7807	-3.2373	1.0151	O	0.2681	-3.254	1.1864
H	2.0491	1.3695	-0.1875	H	2.0491	1.3821	-0.188
H	2.2173	-1.1338	-0.0778	H	2.2173	-1.1212	-0.0783
H	-2.2173	1.0077	0.0792	H	-2.2173	1.0203	0.0787
H	0.8684	3.0534	1.5919	H	-0.1399	2.9825	1.9314
H	0.6144	5.3285	1.4457	H	-0.3644	5.26	1.7752
H	-0.954	-3.048	-1.5919	H	0.0565	-2.9779	-1.9314
H	-0.7571	-5.3285	-1.4419	H	0.2236	-5.26	-1.7713
	120°				**150°**		
C	1.1421	0.7778	-0.1062	C	1.1421	0.787	-0.1066

C	1.2382	-0.6086	-0.0456	C	1.2382	-0.5994	-0.046
C	0.0676	-1.343	0.0579	C	0.0676	-1.3338	0.0575
N	-1.1644	-0.7907	0.1036	N	-1.1644	-0.7815	0.1032
C	-1.226	0.5574	0.0428	C	-1.226	0.5666	0.0424
C	-0.1128	1.3761	-0.0614	C	-0.1128	1.3853	-0.0618
C	0.164	-2.6893	0.1165	C	0.164	-2.6801	0.1161
C	-0.243	2.7196	-0.1179	C	-0.243	2.7288	-0.1183
N	-0.8381	3.3936	0.9146	N	-1.2947	3.3415	0.5086
O	-0.9649	4.7023	0.8596	O	-1.4215	4.6502	0.4536
N	0.7432	-3.3796	-0.9141	N	1.2006	-3.32	-0.5085
O	0.8371	-4.691	-0.8569	O	1.2945	-4.6314	-0.4513
O	0.1657	3.3261	-1.0792	O	0.5684	3.3894	-0.7218
O	-0.261	-3.284	1.0783	O	-0.6646	-3.3193	0.7196
H	2.0491	1.3946	-0.1886	H	2.0491	1.4038	-0.189
H	2.2173	-1.1087	-0.0789	H	2.2173	-1.0995	-0.0793
H	-2.2173	1.0328	0.0781	H	-2.2173	1.042	0.0777
H	-1.1805	2.8854	1.7199	H	-1.9745	2.7879	1.0141
H	-1.3745	5.1661	1.57	H	-2.1452	5.0718	0.8849
H	1.0992	-2.8814	-1.7199	H	1.8948	-2.7845	-1.0141
H	1.2357	-5.1661	-1.5661	H	2.0078	-5.0718	-0.8811
180°				**210°**			
C	1.2106	0.7903	-0.1054	C	1.1645	0.787	-0.1083
C	1.3067	-0.5961	-0.0448	C	1.2606	-0.5994	-0.0477
C	0.1361	-1.3305	0.0587	C	0.09	-1.3338	0.0558
N	-1.0959	-0.7782	0.1044	N	-1.142	-0.7815	0.1015
C	-1.1575	0.5699	0.0436	C	-1.2036	0.5666	0.0407
C	-0.0443	1.3886	-0.0606	C	-0.0904	1.3853	-0.0635
C	0.2325	-2.6768	0.1173	C	0.1864	-2.6801	0.1144
C	-0.1745	2.7321	-0.1171	C	-0.2206	2.7288	-0.12
N	-1.4186	3.3017	-0.0714	N	-1.3415	3.285	-0.6755
O	-1.5455	4.6104	-0.1264	O	-1.4684	4.5937	-0.7305
N	1.4619	-3.2776	0.074	N	1.2922	-3.2636	0.672
O	1.5557	-4.589	0.1312	O	1.386	-4.575	0.7291
O	0.8067	3.4308	-0.2078	O	0.6518	3.4392	0.3196
O	-0.7661	-3.3504	0.2078	O	-0.7032	-3.3691	-0.3253
H	2.1176	1.4071	-0.1878	H	2.0715	1.4038	-0.1907
H	2.2858	-1.0962	-0.0781	H	2.2397	-1.0995	-0.081
H	-2.1488	1.0453	0.0789	H	-2.1949	1.042	0.076
H	-2.2406	2.7164	0.0045	H	-2.0724	2.6898	-1.0438
H	-2.4016	5.0024	-0.0951	H	-2.2397	4.9765	-1.1128
H	2.2984	-2.7132	-0.0018	H	2.0374	-2.6864	1.0404
H	2.4016	-5.0024	0.1014	H	2.1468	-4.9765	1.1128
240°				**270°**			
C	1.1421	0.7778	-0.1078	C	1.1421	0.7653	-0.1073
C	1.2382	-0.6086	-0.0472	C	1.2382	-0.6211	-0.0467

C	0.0676	-1.343	0.0563	C	0.0676	-1.3555	0.0568
N	-1.1644	-0.7907	0.102	N	-1.1644	-0.8032	0.1025
C	-1.226	0.5574	0.0412	C	-1.226	0.5449	0.0417
C	-0.1128	1.3761	-0.063	C	-0.1128	1.3636	-0.0624
C	0.164	-2.6893	0.1149	C	0.164	-2.7018	0.1154
C	-0.243	2.7196	-0.1195	C	-0.243	2.7071	-0.119
N	-0.958	3.2959	-1.135	N	-0.3782	3.3313	-1.3299
O	-1.0849	4.6046	-1.19	O	-0.5051	4.64	-1.385
N	0.8631	-3.2819	1.1319	N	0.2821	-3.3275	1.3274
O	0.9568	-4.5933	1.1889	O	0.3759	-4.639	1.3843
O	0.2713	3.4124	0.7258	O	-0.2402	3.3575	0.8989
O	-0.3665	-3.3702	-0.7302	O	0.1461	-3.3535	-0.9015
H	2.0491	1.3946	-0.1902	H	2.0491	1.3821	-0.1896
H	2.2173	-1.1087	-0.0805	H	2.2173	-1.1212	-0.08
H	-2.2173	1.0328	0.0765	H	-2.2173	1.0203	0.077
H	-1.3888	2.7154	-1.8432	H	-0.3804	2.7863	-2.1826
H	-1.5768	5.0011	-1.8888	H	-0.598	5.0696	-2.2182
H	1.3075	-2.7115	1.8399	H	0.297	-2.7816	2.1794
H	1.4378	-5.0011	1.8888	H	0.4571	-5.0696	2.2182
300°				**330°**			
C	1.1421	0.7528	-0.1067	C	1.1421	0.7436	-0.1064
C	1.2382	-0.6336	-0.0461	C	1.2382	-0.6428	-0.0458
C	0.0676	-1.368	0.0574	C	0.0676	-1.3772	0.0577
N	-1.1644	-0.8157	0.1031	N	-1.1644	-0.8249	0.1034
C	-1.226	0.5324	0.0423	C	-1.226	0.5232	0.0426
C	-0.1128	1.3511	-0.0619	C	-0.1128	1.3419	-0.0616
C	0.164	-2.7143	0.116	C	0.164	-2.7235	0.1163
C	-0.243	2.6946	-0.1184	C	-0.243	2.6854	-0.1181
N	0.2202	3.3819	-1.2081	N	0.6767	3.434	-0.8022
O	0.0933	4.6905	-1.2632	O	0.5499	4.7427	-0.8573
N	-0.3175	-3.3883	1.206	N	-0.7749	-3.4479	0.8004
O	-0.2236	-4.6997	1.263	O	-0.681	-4.7593	0.8573
O	-0.7681	3.2893	0.7924	O	-1.1708	3.2261	0.4349
O	0.6752	-3.3234	-0.7934	O	1.0788	-3.2881	-0.4347
H	2.0491	1.3696	-0.1891	H	2.0491	1.3604	-0.1888
H	2.2173	-1.1337	-0.0794	H	2.2173	-1.1429	-0.0791
H	-2.2173	1.0078	0.0776	H	-2.2173	0.9986	0.0779
H	0.6601	2.8835	-1.9711	H	1.4541	2.9809	-1.2654
H	0.4121	5.1635	-2.013	H	1.1828	5.2578	-1.3279
H	-0.7457	-2.878	1.9678	H	-1.5413	-2.9749	1.262
H	-0.5549	-5.1635	2.013	H	-1.3271	-5.2578	1.3279

Table S19 Cartesian coordinates of the PDDH ligand geometry after counter-rotation of both hydroxamate groups.

0°				30°			
C	1.1421	0.7402	-0.1063	C	1.1421	0.7912	0.2534
C	1.2382	-0.6462	-0.0457	C	1.2382	-0.5952	0.314
C	0.0676	-1.3806	0.0578	C	0.0676	-1.3296	0.4175
N	-1.1644	-0.8283	0.1035	N	-1.1644	-0.7773	0.4632
C	-1.226	0.5198	0.0427	C	-1.226	0.5708	0.4024
C	-0.1128	1.3385	-0.0615	C	-0.1128	1.3895	0.2982
C	0.164	-2.7269	0.1164	C	0.164	-2.6759	0.4761
C	-0.243	2.682	-0.118	C	-0.243	2.733	0.2417
N	0.8692	3.4737	-0.2209	N	0.6767	3.4816	-0.4424
O	0.7424	4.7824	-0.276	O	0.5499	4.7903	-0.4975
N	-0.9677	-3.4904	0.2191	N	-0.8441	-3.4567	-0.0221
O	-0.8737	-4.8018	0.2761	O	-0.7501	-4.7681	0.035
O	-1.3406	3.1847	-0.0778	O	-1.1708	3.2737	0.7947
O	1.2488	-3.257	0.0783	O	1.1397	-3.1908	0.9682
H	2.0491	1.357	-0.1887	H	2.0491	1.408	0.171
H	2.2173	-1.1463	-0.079	H	2.2173	-1.0953	0.2807
H	-2.2173	0.9952	0.078	H	-2.2173	1.0462	0.4377
H	1.7887	3.0525	-0.2545	H	1.4541	3.0285	-0.9056
H	1.5077	5.3272	-0.3467	H	1.1828	5.3054	-0.9682
H	-1.8765	-3.0463	0.251	H	-1.6616	-3.0254	-0.4344
H	-1.6524	-5.3272	0.3467	H	-1.4438	-5.3054	-0.3079
60°				**90°**			
C	1.1421	0.8352	0.393	C	1.1421	0.8605	0.4095
C	1.2382	-0.5512	0.4536	C	1.2382	-0.5259	0.4701
C	0.0676	-1.2856	0.5571	C	0.0676	-1.2603	0.5736
N	-1.1644	-0.7333	0.6028	N	-1.1644	-0.708	0.6193
C	-1.226	0.6148	0.542	C	-1.226	0.6401	0.5585
C	-0.1128	1.4335	0.4378	C	-0.1128	1.4588	0.4543
C	0.164	-2.6319	0.6157	C	0.164	-2.6066	0.6322
C	-0.243	2.777	0.3813	C	-0.243	2.8023	0.3978
N	0.2202	3.4643	-0.7084	N	-0.3782	3.4265	-0.8132
O	0.0933	4.773	-0.7634	O	-0.5051	4.7352	-0.8683
N	-0.4374	-3.4036	-0.3419	N	0.1436	-3.3452	-0.5204
O	-0.3434	-4.715	-0.2848	O	0.2376	-4.6565	-0.4632
O	-0.7681	3.3718	1.2921	O	-0.2402	3.4528	1.4156
O	0.7807	-3.1548	1.5132	O	0.2681	-3.1587	1.7015
H	2.0491	1.452	0.3106	H	2.0491	1.4773	0.3271
H	2.2173	-1.0513	0.4203	H	2.2173	-1.026	0.4368
H	-2.2173	1.0902	0.5773	H	-2.2173	1.1155	0.5938
H	0.6601	2.966	-1.4713	H	-0.3804	2.8816	-1.6659
H	0.4121	5.246	-1.5132	H	-0.598	5.1648	-1.7015
H	-0.954	-2.9655	-1.0938	H	0.0565	-2.8826	-1.4163
H	-0.7571	-5.246	-0.9437	H	0.2236	-5.1648	-1.2562
120°				**150°**			

C	1.1421	0.8603	0.2982	C	1.1645	0.8346	0.0892
C	1.2382	-0.5261	0.3588	C	1.2606	-0.5518	0.1498
C	0.0676	-1.2605	0.4623	C	0.09	-1.2862	0.2533
N	-1.1644	-0.7082	0.508	N	-1.142	-0.7339	0.299
C	-1.226	0.6399	0.4472	C	-1.2036	0.6142	0.2382
C	-0.1128	1.4586	0.343	C	-0.0904	1.4329	0.134
C	0.164	-2.6068	0.5209	C	0.1864	-2.6325	0.3119
C	-0.243	2.8021	0.2865	C	-0.2206	2.7764	0.0775
N	-0.958	3.3783	-0.7289	N	-1.3415	3.3327	-0.478
O	-1.0849	4.687	-0.7839	O	-1.4684	4.6414	-0.533
N	0.7432	-3.2971	-0.5097	N	1.223	-3.2724	-0.3128
O	0.8371	-4.6085	-0.4525	O	1.3168	-4.5838	-0.2556
O	0.2713	3.4949	1.1319	O	0.6518	3.4868	0.517
O	-0.261	-3.2015	1.4827	O	-0.6422	-3.2717	0.9153
H	2.0491	1.4771	0.2158	H	2.0715	1.4514	0.0068
H	2.2173	-1.0262	0.3255	H	2.2397	-1.0519	0.1165
H	-2.2173	1.1153	0.4825	H	-2.1949	1.0896	0.2735
H	-1.3888	2.7979	-1.4371	H	-2.0724	2.7374	-0.8463
H	-1.5768	5.0836	-1.4827	H	-2.2397	5.0241	-0.9153
H	1.0992	-2.7989	-1.3155	H	1.9171	-2.7369	-0.8183
H	1.2357	-5.0836	-1.1617	H	2.0301	-5.0241	-0.6853
180°				**210°**			
C	1.2106	0.7903	-0.1054	C	1.1421	0.7394	-0.303
C	1.3067	-0.5961	-0.0448	C	1.2382	-0.647	-0.2424
C	0.1361	-1.3305	0.0587	C	0.0676	-1.3814	-0.1389
N	-1.0959	-0.7782	0.1044	N	-1.1644	-0.8291	-0.0932
C	-1.1575	0.5699	0.0436	C	-1.226	0.519	-0.154
C	-0.0443	1.3886	-0.0606	C	-0.1128	1.3377	-0.2582
C	0.2325	-2.6768	0.1173	C	0.164	-2.7277	-0.0803
C	-0.1745	2.7321	-0.1171	C	-0.243	2.6812	-0.3147
N	-1.4186	3.3017	-0.0714	N	-1.2947	3.2939	0.3122
O	-1.5455	4.6104	-0.1264	O	-1.4215	4.6026	0.2572
N	1.4619	-3.2776	0.074	N	1.2698	-3.3112	0.4773
O	1.5557	-4.589	0.1312	O	1.3636	-4.6226	0.5344
O	0.8067	3.4308	-0.2078	O	0.5684	3.3418	-0.9181
O	-0.7661	-3.3504	0.2078	O	-0.7255	-3.4167	-0.52
H	2.1176	1.4071	-0.1878	H	2.0491	1.3562	-0.3854
H	2.2858	-1.0962	-0.0781	H	2.2173	-1.1471	-0.2757
H	-2.1488	1.0453	0.0789	H	-2.2173	0.9944	-0.1187
H	-2.2406	2.7164	0.0045	H	-1.9745	2.7403	0.8177
H	-2.4016	5.0024	-0.0951	H	-2.1452	5.0242	0.6885
H	2.2984	-2.7132	-0.0018	H	2.015	-2.734	0.8457
H	2.4016	-5.0024	0.1014	H	2.1245	-5.0242	0.9181
240°				**270°**			
C	1.1421	0.6953	-0.5118	C	1.1421	0.67	-0.6227

C	1.2382	-0.6911	-0.4512	C	1.2382	-0.7164	-0.5621
C	0.0676	-1.4255	-0.3477	C	0.0676	-1.4508	-0.4586
N	-1.1644	-0.8732	-0.302	N	-1.1644	-0.8985	-0.4129
C	-1.226	0.4749	-0.3628	C	-1.226	0.4496	-0.4737
C	-0.1128	1.2936	-0.467	C	-0.1128	1.2683	-0.5779
C	0.164	-2.7718	-0.2891	C	0.164	-2.7971	-0.4
C	-0.243	2.6371	-0.5235	C	-0.243	2.6118	-0.6344
N	-0.8381	3.3111	0.509	N	-0.2397	3.3489	0.5193
O	-0.9649	4.6198	0.454	O	-0.3665	4.6576	0.4643
N	0.8631	-3.3644	0.7279	N	0.2821	-3.4228	0.8119
O	0.9568	-4.6758	0.785	O	0.3759	-4.7342	0.8689
O	0.1657	3.2437	-1.4848	O	-0.3622	3.1627	-1.7028
O	-0.3665	-3.4527	-1.1342	O	0.1461	-3.4487	-1.417
H	2.0491	1.3121	-0.5942	H	2.0491	1.2868	-0.7051
H	2.2173	-1.1912	-0.4845	H	2.2173	-1.2165	-0.5954
H	-2.2173	0.9503	-0.3275	H	-2.2173	0.925	-0.4384
H	-1.1805	2.8029	1.3143	H	-0.1399	2.8873	1.4143
H	-1.3745	5.0836	1.1644	H	-0.3644	5.1648	1.2582
H	1.3075	-2.794	1.4359	H	0.297	-2.8769	1.6639
H	1.4378	-5.0836	1.4848	H	0.4571	-5.1648	1.7028
300°				**330°**			
C	1.1421	0.6703	-0.6061	C	1.1421	0.6959	-0.4662
C	1.2382	-0.7161	-0.5455	C	1.2382	-0.6905	-0.4056
C	0.0676	-1.4505	-0.442	C	0.0676	-1.4249	-0.3021
N	-1.1644	-0.8982	-0.3963	N	-1.1644	-0.8726	-0.2564
C	-1.226	0.4499	-0.4571	C	-1.226	0.4755	-0.3172
C	-0.1128	1.2686	-0.5613	C	-0.1128	1.2942	-0.4214
C	0.164	-2.7968	-0.3834	C	0.164	-2.7712	-0.2435
C	-0.243	2.6121	-0.6178	C	-0.243	2.6377	-0.4779
N	0.3401	3.3971	0.3404	N	0.746	3.4428	0.0203
O	0.2133	4.7058	0.2854	O	0.6192	4.7515	-0.0348
N	-0.3175	-3.4708	0.7067	N	-0.7749	-3.4956	0.4405
O	-0.2236	-4.7822	0.7636	O	-0.681	-4.807	0.4974
O	-0.8737	3.1206	-1.5136	O	-1.2318	3.1287	-0.9681
O	0.6752	-3.4059	-1.2927	O	1.0788	-3.3358	-0.7946
H	2.0491	1.2871	-0.6885	H	2.0491	1.3127	-0.5486
H	2.2173	-1.2162	-0.5788	H	2.2173	-1.1906	-0.4389
H	-2.2173	0.9253	-0.4218	H	-2.2173	0.9509	-0.2819
H	0.8684	2.971	1.0909	H	1.5743	3.0314	0.4309
H	0.6144	5.246	0.9447	H	1.2996	5.3055	0.3081
H	-0.7457	-2.9605	1.4685	H	-1.5413	-3.0225	0.9021
H	-0.5549	-5.246	1.5136	H	-1.3271	-5.3055	0.9681

Table S20 Cartesian coordinates of the rotated geometry for the single-side

hydroxamate group in the H_2-F_2-BDHA ligand model.

0°				**30°**			
C	-0.9243	1.0446	-0.0094	C	-0.9584	1.0446	-0.1671
C	0.4302	1.3137	0.1866	C	0.3961	1.3137	0.0289
C	1.3545	0.2691	0.196	C	1.3204	0.2691	0.0383
C	0.9243	-1.0445	0.0096	C	0.8902	-1.0445	-0.1481
C	-0.4302	-1.3137	-0.1862	C	-0.4643	-1.3137	-0.3439
C	-1.3545	-0.2691	-0.1958	C	-1.3886	-0.2691	-0.3535
C	2.6665	0.5297	0.3857	C	2.6324	0.5297	0.228
C	-2.6665	-0.5297	-0.3855	C	-2.7006	-0.5297	-0.5432
N	-3.5737	0.4955	-0.3949	N	-3.6078	0.4955	-0.5526
O	-4.8517	0.2416	-0.5797	O	-4.8858	0.2416	-0.7374
N	3.5737	-0.4955	0.395	N	3.58	-0.2813	-0.3363
O	4.8517	-0.2416	0.5796	O	4.858	-0.0273	-0.1517
O	-3.0391	-1.6675	-0.547	O	-3.0732	-1.6675	-0.7047
O	3.0391	1.6675	0.5472	O	2.9694	1.4784	0.8958
F	-1.799	2.0331	-0.0184	F	-1.8331	2.0331	-0.1761
F	1.799	-2.033	0.0186	F	1.7649	-2.033	-0.1391
H	0.7695	2.3497	0.3337	H	0.7354	2.3497	0.176
H	-0.7695	-2.3497	-0.3332	H	-0.8036	-2.3497	-0.4909
H	-3.2615	1.4486	-0.2597	H	-3.2956	1.4486	-0.4174
H	-5.4759	0.9471	-0.5861	H	-5.51	0.9471	-0.7438
H	3.2615	-1.4486	0.2596	H	3.2976	-1.0759	-0.8958
H	5.4759	-0.947	0.5861	H	5.51	-0.5854	-0.5399
60°				**90°**			
C	-0.9285	1.0446	0.0028	C	-0.8427	1.0446	0.0514
C	0.426	1.3137	0.1988	C	0.5118	1.3137	0.2474
C	1.3503	0.2691	0.2082	C	1.4361	0.2691	0.2568
C	0.9201	-1.0445	0.0218	C	1.0059	-1.0445	0.0704
C	-0.4344	-1.3137	-0.174	C	-0.3486	-1.3137	-0.1254
C	-1.3587	-0.2691	-0.1836	C	-1.2729	-0.2691	-0.135
C	2.6623	0.5297	0.3979	C	2.7481	0.5297	0.4465
C	-2.6707	-0.5297	-0.3733	C	-2.5849	-0.5297	-0.3247
N	-3.5779	0.4955	-0.3827	N	-3.4921	0.4955	-0.3341
O	-4.8559	0.2416	-0.5675	O	-4.7701	0.2416	-0.5189
N	3.5745	0.1856	-0.5631	N	3.5586	0.7801	-0.628
O	4.8524	0.4396	-0.3784	O	4.8366	1.0341	-0.4431
O	-3.0433	-1.6675	-0.5348	O	-2.9575	-1.6675	-0.4862
O	3.0305	1.0663	1.4158	O	3.206	0.5417	1.5644
F	-1.8032	2.0331	-0.0062	F	-1.7174	2.0331	0.0424
F	1.7948	-2.033	0.0308	F	1.8806	-2.033	0.0794
H	0.7653	2.3497	0.3459	H	0.8511	2.3497	0.3945
H	-0.7737	-2.3497	-0.321	H	-0.6879	-2.3497	-0.2724
H	-3.2657	1.4486	-0.2475	H	-3.1799	1.4486	-0.1989

H	-5.4801	0.9471	-0.5739	H	-5.3943	0.9471	-0.5253
H	3.266	-0.2638	-1.4158	H	3.1749	0.7701	-1.5644
H	5.4801	0.2028	-1.0396	H	5.3943	1.2063	-1.1824
	120°				**150°**		
C	-0.7239	1.0446	-0.0344	C	-0.604	0.8204	-0.1767
C	0.6306	1.3137	0.1616	C	0.7505	1.0895	0.0193
C	1.5549	0.2691	0.171	C	1.6748	0.0449	0.0287
C	1.1247	-1.0445	-0.0154	C	1.2446	-1.2687	-0.1577
C	-0.2298	-1.3137	-0.2112	C	-0.1099	-1.5379	-0.3535
C	-1.1541	-0.2691	-0.2208	C	-1.0342	-0.4933	-0.3631
C	2.8669	0.5297	0.3607	C	2.9868	0.3055	0.2184
C	-2.4661	-0.5297	-0.4105	C	-2.3462	-0.7539	-0.5528
N	-3.3733	0.4955	-0.4199	N	-3.2534	0.2713	-0.5622
O	-4.6513	0.2416	-0.6047	O	-4.5314	0.0174	-0.747
N	3.5367	1.3429	-0.5135	N	3.5145	1.4989	-0.1955
O	4.8146	1.5968	-0.3286	O	4.7925	1.7528	-0.0106
O	-2.8387	-1.6675	-0.572	O	-2.7188	-1.8917	-0.7143
O	3.449	0.045	1.3018	O	3.6943	-0.5147	0.7534
F	-1.5986	2.0331	-0.0434	F	-1.4787	1.8089	-0.1857
F	1.9994	-2.033	-0.0064	F	2.1193	-2.2572	-0.1487
H	0.9699	2.3497	0.3087	H	1.0898	2.1255	0.1664
H	-0.5691	-2.3497	-0.3582	H	-0.4492	-2.5739	-0.5005
H	-3.0611	1.4486	-0.2847	H	-2.9412	1.2244	-0.427
H	-5.2755	0.9471	-0.6111	H	-5.1556	0.7229	-0.7534
H	3.0489	1.7489	-1.3018	H	2.9217	2.186	-0.6436
H	5.2755	2.1563	-0.9302	H	5.1556	2.5739	-0.2955
	180°				**210°**		
C	-0.5151	0.7395	-0.156	C	-0.481	0.9203	-0.6402
C	0.8394	1.0086	0.04	C	0.8735	1.1894	-0.4442
C	1.7637	-0.036	0.0494	C	1.7978	0.1448	-0.4348
C	1.3335	-1.3496	-0.137	C	1.3676	-1.1688	-0.6212
C	-0.021	-1.6188	-0.3328	C	0.0131	-1.438	-0.817
C	-0.9453	-0.5742	-0.3424	C	-0.9112	-0.3934	-0.8266
C	3.0757	0.2246	0.2391	C	3.1098	0.4054	-0.2451
C	-2.2573	-0.8348	-0.5321	C	-2.2232	-0.654	-1.0163
N	-3.1645	0.1904	-0.5415	N	-3.1304	0.3712	-1.0257
O	-4.4425	-0.0635	-0.7263	O	-4.4084	0.1173	-1.2105
N	3.4981	1.5139	0.422	N	3.4918	1.4805	0.5115
O	4.7761	1.7677	0.607	O	4.7698	1.7342	0.6964
O	-2.6299	-1.9726	-0.6936	O	-2.5958	-1.7918	-1.1778
O	3.8762	-0.6802	0.2472	O	3.9459	-0.3103	-0.7433
F	-1.3898	1.728	-0.165	F	-1.3557	1.9088	-0.6492
F	2.2082	-2.3381	-0.128	F	2.2423	-2.1573	-0.6122
H	1.1787	2.0446	0.1871	H	1.2128	2.2254	-0.2971
H	-0.3603	-2.6548	-0.4798	H	-0.3262	-2.474	-0.964

H	-2.8523	1.1435	-0.4063	H	-2.8182	1.3243	-0.8905
H	-5.0667	0.642	-0.7327	H	-5.0326	0.8228	-1.2169
H	2.8274	2.2718	0.4153	H	2.7913	2.0799	0.9288
H	5.0667	2.6548	0.7327	H	5.0326	2.474	1.2169
240°				**270°**			
C	-0.5109	1.0446	-0.975	C	-0.5967	1.0446	-1.0707
C	0.8436	1.3137	-0.779	C	0.7578	1.3137	-0.8747
C	1.7679	0.2691	-0.7696	C	1.6821	0.2691	-0.8653
C	1.3377	-1.0445	-0.956	C	1.2519	-1.0445	-1.0517
C	-0.0168	-1.3137	-1.1518	C	-0.1026	-1.3137	-1.2475
C	-0.9411	-0.2691	-1.1614	C	-1.0269	-0.2691	-1.2571
C	3.0799	0.5297	-0.5799	C	2.9941	0.5297	-0.6756
C	-2.2531	-0.5297	-1.3511	C	-2.3389	-0.5297	-1.4468
N	-3.1603	0.4955	-1.3605	N	-3.2461	0.4955	-1.4562
O	-4.4383	0.2416	-1.5453	O	-4.5241	0.2416	-1.641
N	3.4973	1.1379	0.5734	N	3.5131	0.5434	0.5911
O	4.7753	1.3915	0.7582	O	4.7912	0.7971	0.7758
O	-2.6257	-1.6675	-1.5126	O	-2.7115	-1.6675	-1.6083
O	3.8848	0.2261	-1.4281	O	3.7093	0.7507	-1.6239
F	-1.3856	2.0331	-0.984	F	-1.4714	2.0331	-1.0797
F	2.2124	-2.033	-0.947	F	2.1266	-2.033	-1.0427
H	1.1829	2.3497	-0.6319	H	1.0971	2.3497	-0.7276
H	-0.3561	-2.3497	-1.2988	H	-0.4419	-2.3497	-1.3945
H	-2.8481	1.4486	-1.2253	H	-2.9339	1.4486	-1.321
H	-5.0625	0.9471	-1.5517	H	-5.1483	0.9471	-1.6474
H	2.823	1.3921	1.2839	H	2.914	0.3581	1.3854
H	5.0625	1.8101	1.5517	H	5.1483	0.8066	1.6474
300°				**330°**			
C	-0.7155	1.0446	-0.9017	C	-0.8354	1.0446	-0.5132
C	0.639	1.3137	-0.7057	C	0.5191	1.3137	-0.3172
C	1.5633	0.2691	-0.6963	C	1.4434	0.2691	-0.3078
C	1.1331	-1.0445	-0.8827	C	1.0132	-1.0445	-0.4942
C	-0.2214	-1.3137	-1.0785	C	-0.3413	-1.3137	-0.69
C	-1.1457	-0.2691	-1.0881	C	-1.2656	-0.2691	-0.6996
C	2.8753	0.5297	-0.5066	C	2.7554	0.5297	-0.1181
C	-2.4577	-0.5297	-1.2778	C	-2.5776	-0.5297	-0.8893
N	-3.3649	0.4955	-1.2872	N	-3.4848	0.4955	-0.8987
O	-4.6429	0.2416	-1.472	O	-4.7628	0.2416	-1.0835
N	3.5351	-0.0194	0.5599	N	3.5573	-0.3996	0.4881
O	4.8131	0.2343	0.7445	O	4.8353	-0.1458	0.6727
O	-2.8303	-1.6675	-1.4393	O	-2.9502	-1.6675	-1.0508
O	3.4663	1.2474	-1.2781	O	3.221	1.5829	-0.4834
F	-1.5902	2.0331	-0.9107	F	-1.7101	2.0331	-0.5222
F	2.0078	-2.033	-0.8737	F	1.8879	-2.033	-0.4852
H	0.9783	2.3497	-0.5586	H	0.8584	2.3497	-0.1701

H	-0.5607	-2.3497	-1.2255	H	-0.6806	-2.3497	-0.837
H	-3.0527	1.4486	-1.152	H	-3.1726	1.4486	-0.7635
H	-5.2671	0.9471	-1.4784	H	-5.387	0.9471	-1.0899
H	3.04	-0.6206	1.2061	H	3.1672	-1.2819	0.794
H	5.2671	-0.1434	1.4784	H	5.387	-0.7852	1.0899

Table S21 Cartesian coordinates of the H_2-F_2-BDHA ligand geometry after co-rotation of both hydroxamate groups.

0°				**30°**			
C	-0.9243	1.0446	-0.0094	C	-1.0473	1.0446	0.2609
C	0.4302	1.3137	0.1866	C	0.3072	1.3137	0.4568
C	1.3545	0.2691	0.196	C	1.2315	0.2691	0.4663
C	0.9243	-1.0445	0.0096	C	0.8012	-1.0445	0.2799
C	-0.4302	-1.3137	-0.1862	C	-0.5532	-1.3137	0.084
C	-1.3545	-0.2691	-0.1958	C	-1.4776	-0.2691	0.0745
C	2.6665	0.5297	0.3857	C	2.5435	0.5297	0.6559
C	-2.6665	-0.5297	-0.3855	C	-2.7895	-0.5297	-0.1153
N	-3.5737	0.4955	-0.3949	N	-3.5913	0.3997	-0.7216
O	-4.8517	0.2416	-0.5797	O	-4.8693	0.1458	-0.9064
N	3.5737	-0.4955	0.395	N	3.491	-0.2813	0.0915
O	4.8517	-0.2416	0.5796	O	4.769	-0.0274	0.2763
O	-3.0391	-1.6675	-0.547	O	-3.2552	-1.5828	0.2501
O	3.0391	1.6675	0.5472	O	2.8804	1.4784	1.3236
F	-1.799	2.0331	-0.0184	F	-1.9221	2.0331	0.2518
F	1.799	-2.033	0.0186	F	1.676	-2.033	0.2888
H	0.7695	2.3497	0.3337	H	0.6464	2.3497	0.6039
H	-0.7695	-2.3497	-0.3332	H	-0.8925	-2.3497	-0.0629
H	-3.2615	1.4486	-0.2597	H	-3.2013	1.2819	-1.0276
H	-5.4759	0.9471	-0.5861	H	-5.421	0.7853	-1.3236
H	3.2615	-1.4486	0.2596	H	3.2087	-1.076	-0.4678
H	5.4759	-0.947	0.5861	H	5.421	-0.5854	-0.1121
60°				**90°**			
C	-1.1374	1.0446	0.4743	C	-1.1704	1.0446	0.5933
C	0.2171	1.3137	0.6703	C	0.1841	1.3137	0.7893
C	1.1414	0.2691	0.6797	C	1.1084	0.2691	0.7987
C	0.7112	-1.0445	0.4933	C	0.6782	-1.0445	0.6123
C	-0.6433	-1.3137	0.2975	C	-0.6763	-1.3137	0.4164
C	-1.5676	-0.2691	0.288	C	-1.6006	-0.2691	0.4069
C	2.4534	0.5297	0.8694	C	2.4204	0.5297	0.9884
C	-2.8796	-0.5297	0.0982	C	-2.9126	-0.5297	0.2172
N	-3.5393	0.0194	-0.9683	N	-3.4315	-0.5434	-1.0496
O	-4.8173	-0.2345	-1.1532	O	-4.7095	-0.7973	-1.2345
N	3.3655	0.1857	-0.0917	N	3.2309	0.7802	-0.0862

O	4.6435	0.4395	0.093	O	4.5089	1.034	0.0986
O	-3.4706	-1.2472	0.8696	O	-3.6278	-0.7506	1.1653
O	2.8216	1.0664	1.8871	O	2.8784	0.5418	2.1061
F	-2.0121	2.0331	0.4653	F	-2.0451	2.0331	0.5843
F	1.5859	-2.033	0.5023	F	1.5529	-2.033	0.6213
H	0.5564	2.3497	0.8174	H	0.5234	2.3497	0.9363
H	-0.9826	-2.3497	0.1505	H	-1.0156	-2.3497	0.2695
H	-3.0442	0.6205	-1.6146	H	-2.8323	-0.3583	-1.8439
H	-5.2712	0.1433	-1.8871	H	-5.0665	-0.8067	-2.1061
H	3.0571	-0.2639	-0.9443	H	2.8472	0.77	-1.0226
H	5.2712	0.2028	-0.5683	H	5.0665	1.2064	-0.6408
	120°				**150°**		
C	-1.1374	1.0446	0.5859	C	-1.0473	0.9447	0.4541
C	0.2171	1.3137	0.7819	C	0.3072	1.2138	0.6501
C	1.1414	0.2691	0.7913	C	1.2315	0.1692	0.6595
C	0.7112	-1.0445	0.6049	C	0.8012	-1.1444	0.4731
C	-0.6433	-1.3137	0.4091	C	-0.5532	-1.4136	0.2773
C	-1.5676	-0.2691	0.3995	C	-1.4776	-0.369	0.2678
C	2.4534	0.5297	0.981	C	2.5435	0.4298	0.8492
C	-2.8796	-0.5297	0.2098	C	-2.7895	-0.6296	0.078
N	-3.2968	-1.1379	-0.9436	N	-3.1714	-1.7047	-0.6786
O	-4.5748	-1.3918	-1.1284	O	-4.4494	-1.9586	-0.8635
N	3.1231	1.3429	0.1067	N	3.0711	1.6233	0.4352
O	4.4011	1.5968	0.2914	O	4.3491	1.8772	0.6199
O	-3.6846	-0.2261	1.0578	O	-3.6257	0.086	0.576
O	3.0356	0.0452	1.922	O	3.251	-0.3902	1.3841
F	-2.0121	2.0331	0.5769	F	-1.9221	1.9332	0.4451
F	1.5859	-2.033	0.6139	F	1.676	-2.133	0.4821
H	0.5564	2.3497	0.9289	H	0.6464	2.2498	0.7972
H	-0.9826	-2.3497	0.2621	H	-0.8925	-2.4496	0.1303
H	-2.6225	-1.3923	-1.654	H	-2.4709	-2.3043	-1.0958
H	-4.8619	-1.8103	-1.922	H	-4.7121	-2.6984	-1.3841
H	2.6354	1.7489	-0.6817	H	2.4783	2.3103	-0.0129
H	4.8619	2.1564	-0.3101	H	4.7121	2.6984	0.3351
	180°				**210°**		
C	-0.9243	1.0446	-0.0094	C	-0.8013	1.1444	-0.473
C	0.4302	1.3137	0.1865	C	0.5532	1.4136	-0.277
C	1.3545	0.2691	0.196	C	1.4775	0.369	-0.2676
C	0.9243	-1.0446	0.0096	C	1.0473	-0.9447	-0.454
C	-0.4302	-1.3137	-0.1863	C	-0.3072	-1.2138	-0.6498
C	-1.3545	-0.2691	-0.1958	C	-1.2315	-0.1692	-0.6593
C	2.6665	0.5297	0.3856	C	2.7895	0.6296	-0.0779
C	-2.6665	-0.5297	-0.3856	C	-2.5435	-0.4298	-0.8491
N	-3.0888	-1.8191	-0.5685	N	-3.0711	-1.6233	-0.4351
O	-4.3668	-2.0729	-0.7533	O	-4.3491	-1.8772	-0.62

N	3.0888	1.8191	0.5686	N	3.1714	1.7047	0.6787
O	4.3668	2.0729	0.7533	O	4.4494	1.9586	0.8635
O	-3.467	0.3749	-0.3938	O	-3.251	0.3902	-1.3841
O	3.467	-0.3749	0.3938	O	3.6256	-0.086	-0.5759
F	-1.799	2.0331	-0.0184	F	-1.676	2.133	-0.482
F	1.799	-2.0331	0.0185	F	1.922	-1.9332	-0.445
H	0.7695	2.3497	0.3336	H	0.8925	2.4496	-0.1299
H	-0.7695	-2.3497	-0.3332	H	-0.6465	-2.2498	-0.7967
H	-2.4182	-2.5769	-0.5616	H	-2.4784	-2.3103	0.0131
H	-4.6573	-2.9601	-0.8792	H	-4.7122	-2.6984	-0.3351
H	2.4182	2.5769	0.5617	H	2.471	2.3042	1.096
H	4.6573	2.9601	0.8792	H	4.7122	2.6984	1.3841
240°				**270°**			
C	-0.7112	1.0446	-0.6047	C	-0.6782	1.0446	-0.6121
C	0.6433	1.3137	-0.4088	C	0.6763	1.3137	-0.4162
C	1.5676	0.2691	-0.3993	C	1.6006	0.2691	-0.4067
C	1.1374	-1.0445	-0.5857	C	1.1703	-1.0445	-0.5931
C	-0.2171	-1.3137	-0.7816	C	-0.1841	-1.3137	-0.789
C	-1.1414	-0.2691	-0.7911	C	-1.1085	-0.2691	-0.7985
C	2.8796	0.5297	-0.2097	C	2.9126	0.5297	-0.2171
C	-2.4534	-0.5297	-0.9809	C	-2.4205	-0.5297	-0.9883
N	-3.1232	-1.3429	-0.1066	N	-3.231	-0.7801	0.0862
O	-4.4012	-1.5968	-0.2915	O	-4.509	-1.034	-0.0986
N	3.2969	1.1379	0.9436	N	3.4316	0.5434	1.0497
O	4.5749	1.3918	1.1284	O	4.7096	0.7973	1.2344
O	-3.0355	-0.0452	-1.922	O	-2.8783	-0.5418	-2.1061
O	3.6845	0.2261	-1.0578	O	3.6277	0.7507	-1.1652
F	-1.5859	2.0331	-0.6138	F	-1.553	2.0331	-0.6212
F	2.0121	-2.033	-0.5768	F	2.0451	-2.033	-0.5842
H	0.9826	2.3497	-0.2617	H	1.0155	2.3497	-0.2691
H	-0.5564	-2.3497	-0.9285	H	-0.5234	-2.3497	-0.9359
H	-2.6355	-1.7488	0.6818	H	-2.8474	-0.77	1.0226
H	-4.862	-2.1563	0.3101	H	-5.0667	-1.2063	0.6407
H	2.6226	1.3923	1.6541	H	2.8325	0.3583	1.844
H	4.862	1.8103	1.922	H	5.0667	0.8067	2.1061
300°				**330°**			
C	-0.7112	1.0446	-0.4931	C	-0.7112	1.0446	-0.4931
C	0.6433	1.3137	-0.2972	C	0.6433	1.3137	-0.2972
C	1.5676	0.2691	-0.2878	C	1.5676	0.2691	-0.2878
C	1.1374	-1.0445	-0.4741	C	1.1374	-1.0445	-0.4741
C	-0.2171	-1.3137	-0.67	C	-0.2171	-1.3137	-0.67
C	-1.1414	-0.2691	-0.6795	C	-1.1414	-0.2691	-0.6795
C	2.8796	0.5297	-0.0981	C	2.8796	0.5297	-0.0981
C	-2.4534	-0.5297	-0.8693	C	-2.4534	-0.5297	-0.8693
N	-3.3656	-0.1856	0.0918	N	-3.3656	-0.1856	0.0918

O	-4.6436	-0.4395	-0.0931	O	-4.6436	-0.4395	-0.0931
N	3.5394	-0.0194	0.9684	N	3.5394	-0.0194	0.9684
O	4.8173	0.2345	1.1531	O	4.8173	0.2345	1.1531
O	-2.8216	-1.0664	-1.887	O	-2.8216	-1.0664	-1.887
O	3.4705	1.2473	-0.8695	O	3.4705	1.2473	-0.8695
F	-1.5859	2.0331	-0.5022	F	-1.5859	2.0331	-0.5022
F	2.0121	-2.033	-0.4652	F	2.0121	-2.033	-0.4652
H	0.9826	2.3497	-0.1501	H	0.9826	2.3497	-0.1501
H	-0.5564	-2.3497	-0.8169	H	-0.5564	-2.3497	-0.8169
H	-3.0572	0.264	0.9443	H	-3.0572	0.264	0.9443
H	-5.2713	-0.2027	0.5682	H	-5.2713	-0.2027	0.5682
H	3.0443	-0.6205	1.6147	H	3.0443	-0.6205	1.6147
H	5.2713	-0.1433	1.887	H	5.2713	-0.1433	1.887

Table S22 Cartesian coordinates of the H_2-F_2-BDHA ligand geometry after counter-rotation of both hydroxamate groups.

0°				**30°**			
C	-0.9243	1.0446	-0.0094	C	-0.9243	1.0446	-0.0094
C	0.4302	1.3137	0.1866	C	0.4302	1.3137	0.1866
C	1.3545	0.2691	0.196	C	1.3545	0.2691	0.196
C	0.9243	-1.0445	0.0096	C	0.9243	-1.0445	0.0096
C	-0.4302	-1.3137	-0.1862	C	-0.4302	-1.3137	-0.1862
C	-1.3545	-0.2691	-0.1958	C	-1.3545	-0.2691	-0.1958
C	2.6665	0.5297	0.3857	C	2.6665	0.5297	0.3857
C	-2.6665	-0.5297	-0.3855	C	-2.6665	-0.5297	-0.3855
N	-3.5737	0.4955	-0.3949	N	-3.4684	0.3996	-0.9918
O	-4.8517	0.2416	-0.5797	O	-4.7464	0.1457	-1.1766
N	3.5737	-0.4955	0.395	N	3.4683	-0.3996	0.9919
O	4.8517	-0.2416	0.5796	O	4.7464	-0.1458	1.1765
O	-3.0391	-1.6675	-0.547	O	-3.1321	-1.5829	-0.0202
O	3.0391	1.6675	0.5472	O	3.1321	1.5829	0.0204
F	-1.799	2.0331	-0.0184	F	-1.799	2.0331	-0.0184
F	1.799	-2.033	0.0186	F	1.799	-2.033	0.0186
H	0.7695	2.3497	0.3337	H	0.7695	2.3497	0.3337
H	-0.7695	-2.3497	-0.3332	H	-0.7695	-2.3497	-0.3332
H	-3.2615	1.4486	-0.2597	H	-3.0783	1.2818	-1.2979
H	-5.4759	0.9471	-0.5861	H	-5.2981	0.7852	-1.5937
H	3.2615	-1.4486	0.2596	H	3.0783	-1.2819	1.2978
H	5.4759	-0.947	0.5861	H	5.2981	-0.7852	1.5937
60°				**90°**			
C	-0.9243	1.0446	-0.0094	C	-0.9243	1.0446	-0.0095
C	0.4302	1.3137	0.1866	C	0.4302	1.3137	0.1865
C	1.3545	0.2691	0.196	C	1.3545	0.2691	0.1959

C	0.9243	-1.0445	0.0096	C	0.9243	-1.0445	0.0095
C	-0.4302	-1.3137	-0.1862	C	-0.4302	-1.3137	-0.1863
C	-1.3545	-0.2691	-0.1958	C	-1.3545	-0.2691	-0.1959
C	2.6665	0.5297	0.3857	C	2.6665	0.5297	0.3856
C	-2.6665	-0.5297	-0.3855	C	-2.6665	-0.5297	-0.3856
N	-3.3263	0.0193	-1.452	N	-3.1856	-0.5435	-1.6523
O	-4.6043	-0.2346	-1.6368	O	-4.4636	-0.7974	-1.837
N	3.3263	-0.0194	1.4522	N	3.1855	0.5434	1.6524
O	4.6043	0.2343	1.6368	O	4.4635	0.7971	1.8371
O	-3.2575	-1.2474	0.386	O	-3.3817	-0.7507	0.5627
O	3.2574	1.2474	-0.3858	O	3.3816	0.7507	-0.5626
F	-1.799	2.0331	-0.0184	F	-1.799	2.0331	-0.0185
F	1.799	-2.033	0.0186	F	1.799	-2.033	0.0185
H	0.7695	2.3497	0.3337	H	0.7695	2.3497	0.3336
H	-0.7695	-2.3497	-0.3332	H	-0.7695	-2.3497	-0.3333
H	-2.8312	0.6204	-2.0983	H	-2.5864	-0.3584	-2.4466
H	-5.0582	0.1432	-2.3706	H	-4.8207	-0.8068	-2.7087
H	2.8312	-0.6206	2.0984	H	2.5864	0.3581	2.4467
H	5.0582	-0.1434	2.3706	H	4.8207	0.8066	2.7087
120°				**150°**			
C	-0.9243	1.0446	-0.0095	C	-0.9243	1.0447	-0.0096
C	0.4302	1.3137	0.1865	C	0.4302	1.3138	0.1864
C	1.3545	0.2691	0.1959	C	1.3545	0.2692	0.1958
C	0.9243	-1.0445	0.0095	C	0.9243	-1.0444	0.0094
C	-0.4302	-1.3137	-0.1863	C	-0.4302	-1.3136	-0.1864
C	-1.3545	-0.2691	-0.1959	C	-1.3545	-0.269	-0.196
C	2.6665	0.5297	0.3856	C	2.6665	0.5298	0.3855
C	-2.6665	-0.5297	-0.3856	C	-2.6665	-0.5296	-0.3857
N	-3.0839	-1.138	-1.5388	N	-3.0485	-1.6047	-1.1422
O	-4.3619	-1.3918	-1.7236	O	-4.3265	-1.8585	-1.3269
N	3.0838	1.1379	1.5389	N	3.0485	1.6049	1.1421
O	4.3619	1.3915	1.7237	O	4.3265	1.8586	1.3271
O	-3.4714	-0.2261	0.4626	O	-3.5026	0.1861	0.1125
O	3.4714	0.2261	-0.4626	O	3.5026	-0.1859	-0.1126
F	-1.799	2.0331	-0.0185	F	-1.799	2.0332	-0.0186
F	1.799	-2.033	0.0185	F	1.799	-2.0329	0.0184
H	0.7695	2.3497	0.3336	H	0.7695	2.3498	0.3335
H	-0.7695	-2.3497	-0.3333	H	-0.7695	-2.3496	-0.3334
H	-2.4096	-1.3924	-2.2493	H	-2.348	-2.2043	-1.5594
H	-4.649	-1.8103	-2.5172	H	-4.5893	-2.5983	-1.8476
H	2.4095	1.3921	2.2494	H	2.348	2.2043	1.5595
H	4.649	1.8101	2.5172	H	4.5893	2.5983	1.8476
180°				**210°**			
C	-0.9243	1.0447	-0.0096	C	-0.9243	1.0446	-0.0095
C	0.4302	1.3138	0.1864	C	0.4302	1.3137	0.1865

C	1.3545	0.2692	0.1958	C	1.3545	0.2691	0.1959
C	0.9243	-1.0444	0.0094	C	0.9243	-1.0445	0.0095
C	-0.4302	-1.3136	-0.1864	C	-0.4302	-1.3137	-0.1863
C	-1.3545	-0.269	-0.196	C	-1.3545	-0.2691	-0.1959
C	2.6665	0.5298	0.3855	C	2.6665	0.5297	0.3856
C	-2.6665	-0.5296	-0.3857	C	-2.6665	-0.5297	-0.3856
N	-3.0889	-1.8189	-0.5685	N	-3.1942	-1.7231	0.0285
O	-4.3669	-2.0727	-0.7533	O	-4.4723	-1.9769	-0.1563
N	3.0889	1.819	0.5684	N	3.1942	1.7231	-0.0284
O	4.3668	2.0728	0.7534	O	4.4722	1.977	0.1566
O	-3.467	0.3751	-0.3938	O	-3.374	0.2905	-0.9205
O	3.467	-0.375	0.3936	O	3.374	-0.2905	0.9205
F	-1.799	2.0332	-0.0186	F	-1.799	2.0331	-0.0185
F	1.799	-2.0329	0.0184	F	1.799	-2.033	0.0185
H	0.7695	2.3498	0.3335	H	0.7695	2.3497	0.3336
H	-0.7695	-2.3496	-0.3334	H	-0.7695	-2.3497	-0.3333
H	-2.4183	-2.5768	-0.5616	H	-2.6015	-2.4101	0.4766
H	-4.6575	-2.9599	-0.8792	H	-4.8353	-2.7981	0.1286
H	2.4182	2.5769	0.5617	H	2.6015	2.4102	-0.4764
H	4.6575	2.9599	0.8792	H	4.8353	2.7981	-0.1283
240°				**270°**			
C	-0.9243	1.0446	-0.0095	C	-0.9243	1.0446	-0.0095
C	0.4302	1.3137	0.1865	C	0.4302	1.3137	0.1865
C	1.3545	0.2691	0.1959	C	1.3545	0.2691	0.1959
C	0.9243	-1.0445	0.0095	C	0.9243	-1.0445	0.0095
C	-0.4302	-1.3137	-0.1863	C	-0.4302	-1.3137	-0.1863
C	-1.3545	-0.2691	-0.1959	C	-1.3545	-0.2691	-0.1959
C	2.6665	0.5297	0.3856	C	2.6665	0.5297	0.3856
C	-2.6665	-0.5297	-0.3856	C	-2.6665	-0.5297	-0.3856
N	-3.3363	-1.3428	0.4887	N	-3.477	-0.78	0.6889
O	-4.6143	-1.5966	0.3038	O	-4.755	-1.0338	0.504
N	3.3363	1.3429	-0.4886	N	3.4771	0.7801	-0.6889
O	4.6143	1.5968	-0.3037	O	4.755	1.0341	-0.504
O	-3.2486	-0.045	-1.3267	O	-3.1244	-0.5417	-1.5035
O	3.2487	0.045	1.3267	O	3.1245	0.5417	1.5035
F	-1.799	2.0331	-0.0185	F	-1.799	2.0331	-0.0185
F	1.799	-2.033	0.0185	F	1.799	-2.033	0.0185
H	0.7695	2.3497	0.3336	H	0.7695	2.3497	0.3336
H	-0.7695	-2.3497	-0.3333	H	-0.7695	-2.3497	-0.3333
H	-2.8486	-1.7487	1.2771	H	-3.0934	-0.7699	1.6253
H	-5.0752	-2.1561	0.9055	H	-5.3127	-1.2061	1.2434
H	2.8486	1.7489	-1.2769	H	3.0933	0.7701	-1.6253
H	5.0752	2.1563	-0.9053	H	5.3127	1.2063	-1.2433
300°				**330°**			
C	-0.9243	1.0446	-0.0094	C	0.4302	1.3137	0.1865

C	0.4302	1.3137	0.1866	C	1.3545	0.2691	0.1959
C	1.3545	0.2691	0.196	C	0.9243	-1.0445	0.0095
C	0.9243	-1.0445	0.0096	C	-0.4302	-1.3137	-0.1863
C	-0.4302	-1.3137	-0.1862	C	-1.3545	-0.2691	-0.1959
C	-1.3545	-0.2691	-0.1958	C	2.6665	0.5297	0.3856
C	2.6665	0.5297	0.3857	C	-2.6665	-0.5297	-0.3856
C	-2.6665	-0.5297	-0.3855	N	-3.6141	0.2813	0.1787
N	-3.5787	-0.1855	0.5755	O	-4.8921	0.0274	-0.0062
O	-4.8567	-0.4394	0.3906	N	3.6141	-0.2813	-0.1788
N	3.5787	0.1856	-0.5754	O	4.8921	-0.0273	0.0059
O	4.8567	0.4396	-0.3906	O	-3.0034	-1.4784	-1.0534
O	-3.0347	-1.0663	-1.4033	O	3.0035	1.4784	1.0534
O	3.0347	1.0663	1.4035	F	-1.799	2.0331	-0.0185
F	-1.799	2.0331	-0.0184	F	1.799	-2.033	0.0185
F	1.799	-2.033	0.0186	H	0.7695	2.3497	0.3336
H	0.7695	2.3497	0.3337	H	-0.7695	-2.3497	-0.3333
H	-0.7695	-2.3497	-0.3332	H	-3.3318	1.0761	0.738
H	-3.2702	0.2641	1.428	H	-5.5441	0.5855	0.3822
H	-5.4844	-0.2026	1.052	H	3.3317	-1.0759	-0.7382
H	3.2702	-0.2638	-1.428	H	5.5441	-0.5854	-0.3823
H	5.4844	0.2028	-1.0518	C	0.4302	1.3137	0.1865

Table S23 Cartesian coordinates of the rotated geometry for the single-side hydroxamate group in the H_2-Cl_2-BDHA ligand model.

0°				**30°**			
C	1.3291	-0.357	-0.2273	C	1.2257	-0.3219	-0.7062
C	0.9954	0.9771	0.0058	C	0.892	1.0122	-0.4731
C	-0.3337	1.3341	0.2331	C	-0.4371	1.3692	-0.2458
C	-1.3291	0.357	0.2271	C	-1.4325	0.3921	-0.2518
C	-0.9954	-0.9771	-0.0061	C	-1.0988	-0.942	-0.485
C	0.3337	-1.3341	-0.2333	C	0.2303	-1.299	-0.7122
C	-0.6569	2.6263	0.459	C	-0.7603	2.6614	-0.0199
C	0.6569	-2.6263	-0.4591	C	0.5535	-2.5912	-0.938
N	1.9613	-2.9767	-0.6821	N	1.8579	-2.9416	-1.161
O	2.2762	-4.2353	-0.9021	O	2.1728	-4.2002	-1.381
N	-1.9614	2.9767	0.682	N	-1.8346	2.9702	0.7705
O	-2.2762	4.2354	0.9021	O	-2.1494	4.2289	0.9906
O	-0.2051	-3.4725	-0.4643	O	-0.3085	-3.4374	-0.9432
O	0.2052	3.4725	0.4641	O	-0.1014	3.5443	-0.5155
Cl	2.967	-0.797	-0.5073	Cl	2.8636	-0.7619	-0.9862
Cl	-2.967	0.797	0.5072	Cl	-3.0704	0.8321	0.0283
H	1.7804	1.7477	0.0104	H	1.677	1.7828	-0.4685
H	-1.7805	-1.7476	-0.0108	H	-1.8839	-1.7125	-0.4897
H	2.6835	-2.2678	-0.6779	H	2.5801	-2.2327	-1.1568

H	3.1738	-4.4764	-1.0555	H	3.0704	-4.4413	-1.5344
H	-2.6835	2.2678	0.6777	H	-2.3865	2.2306	1.1856
H	-3.1738	4.4764	1.0555	H	-2.8886	4.4413	1.5344
	60°				**90°**		
C	1.2257	-0.365	-1.0322	C	1.2257	-0.4748	-1.118
C	0.892	0.9691	-0.7991	C	0.892	0.8593	-0.8849
C	-0.4371	1.3261	-0.5718	C	-0.4371	1.2163	-0.6576
C	-1.4325	0.349	-0.5778	C	-1.4325	0.2392	-0.6636
C	-1.0988	-0.9851	-0.811	C	-1.0988	-1.0949	-0.8968
C	0.2303	-1.3421	-1.0382	C	0.2303	-1.4519	-1.124
C	-0.7603	2.6183	-0.3459	C	-0.7603	2.5085	-0.4317
C	0.5535	-2.6343	-1.264	C	0.5535	-2.7441	-1.3498
N	1.8579	-2.9847	-1.487	N	1.8579	-3.0945	-1.5728
O	2.1728	-4.2433	-1.707	O	2.1728	-4.3531	-1.7928
N	-1.3604	2.9782	0.8307	N	-0.7693	2.9985	0.8466
O	-1.6752	4.2369	1.0508	O	-1.0841	4.2572	1.0666
O	-0.3085	-3.4805	-1.2692	O	-0.3085	-3.5903	-1.355
O	-0.5198	3.4561	-1.1823	O	-1.0414	3.2316	-1.3577
Cl	2.8636	-0.805	-1.3122	Cl	2.8636	-0.9148	-1.398
Cl	-3.0704	0.789	-0.2977	Cl	-3.0704	0.6792	-0.3835
H	1.677	1.7397	-0.7945	H	1.677	1.6299	-0.8803
H	-1.8839	-1.7556	-0.8157	H	-1.8839	-1.8654	-0.9015
H	2.5801	-2.2758	-1.4828	H	2.5801	-2.3856	-1.5686
H	3.0704	-4.4844	-1.8604	H	3.0704	-4.5942	-1.9462
H	-1.5619	2.2763	1.5313	H	-0.5339	2.3927	1.6222
H	-2.0882	4.4844	1.8604	H	-1.0903	4.5942	1.9462
	120°				**150°**		
C	1.2257	-0.6218	-0.9406	C	1.2257	-0.7667	-0.5475
C	0.892	0.7123	-0.7075	C	0.892	0.5674	-0.3144
C	-0.4371	1.0693	-0.4802	C	-0.4371	0.9244	-0.0871
C	-1.4325	0.0922	-0.4862	C	-1.4325	-0.0527	-0.0931
C	-1.0988	-1.2419	-0.7194	C	-1.0988	-1.3868	-0.3263
C	0.2303	-1.5989	-0.9466	C	0.2303	-1.7438	-0.5535
C	-0.7603	2.3615	-0.2543	C	-0.7603	2.2166	0.1388
C	0.5535	-2.8911	-1.1724	C	0.5535	-3.036	-0.7793
N	1.8579	-3.2415	-1.3954	N	1.8579	-3.3864	-1.0023
O	2.1728	-4.5001	-1.6154	O	2.1728	-4.645	-1.2223
N	-0.2197	3.0256	0.8138	N	0.1412	3.0524	0.7412
O	-0.5345	4.2843	1.0338	O	-0.1736	4.3111	0.9612
O	-0.3085	-3.7373	-1.1776	O	-0.3085	-3.8822	-0.7845
O	-1.5264	2.9308	-0.9948	O	-1.8448	2.6344	-0.1907
Cl	2.8636	-1.0618	-1.2206	Cl	2.8636	-1.2067	-0.8275
Cl	-3.0704	0.5322	-0.2061	Cl	-3.0704	0.3873	0.187
H	1.677	1.4829	-0.7029	H	1.677	1.338	-0.3098
H	-1.8839	-2.0124	-0.7241	H	-1.8839	-2.1573	-0.331

H	2.5801	-2.5326	-1.3912	H	2.5801	-2.6775	-0.9981
H	3.0704	-4.7412	-1.7688	H	3.0704	-4.8861	-1.3757
H	0.422	2.5487	1.4341	H	1.0497	2.7023	1.0172
H	-0.1625	4.7412	1.7688	H	0.4468	4.8861	1.3757
180°				**210°**			
C	1.2257	-0.7667	-0.5475	C	1.2257	-0.9058	-0.2778
C	0.892	0.5674	-0.3144	C	0.892	0.4283	-0.0447
C	-0.4371	0.9244	-0.0871	C	-0.4371	0.7853	0.1826
C	-1.4325	-0.0527	-0.0931	C	-1.4325	-0.1918	0.1766
C	-1.0988	-1.3868	-0.3263	C	-1.0988	-1.5259	-0.0566
C	0.2303	-1.7438	-0.5535	C	0.2303	-1.8829	-0.2838
C	-0.7603	2.2166	0.1388	C	-0.7603	2.0775	0.4085
C	0.5535	-3.036	-0.7793	C	0.5535	-3.1751	-0.5096
N	1.8579	-3.3864	-1.0023	N	1.8579	-3.5255	-0.7326
O	2.1728	-4.645	-1.2223	O	2.1728	-4.7841	-0.9526
N	0.1412	3.0524	0.7412	N	-0.0135	3.0781	-0.153
O	-0.1736	4.3111	0.9612	O	-0.3284	4.3368	0.067
O	-0.3085	-3.8822	-0.7845	O	-0.3085	-4.0213	-0.5148
O	-1.8448	2.6344	-0.1907	O	-1.7082	2.3499	1.106
Cl	2.8636	-1.2067	-0.8275	Cl	2.8636	-1.3458	-0.5578
Cl	-3.0704	0.3873	0.187	Cl	-3.0704	0.2482	0.4567
H	1.677	1.338	-0.3098	H	1.677	1.1989	-0.0401
H	-1.8839	-2.1573	-0.331	H	-1.8839	-2.2964	-0.0613
H	2.5801	-2.6775	-0.9981	H	2.5801	-2.8166	-0.7284
H	3.0704	-4.8861	-1.3757	H	3.0704	-5.0252	-1.106
H	1.0497	2.7023	1.0172	H	0.7805	2.8498	-0.7373
H	0.4468	4.8861	1.3757	H	0.1856	5.0252	-0.3194
240°				**270°**			
C	1.2257	-0.8627	-0.2967	C	1.2257	-0.7529	-0.2532
C	0.892	0.4714	-0.0636	C	0.892	0.5812	-0.0201
C	-0.4371	0.8284	0.1637	C	-0.4371	0.9382	0.2072
C	-1.4325	-0.1487	0.1577	C	-1.4325	-0.0389	0.2012
C	-1.0988	-1.4828	-0.0755	C	-1.0988	-1.373	-0.032
C	0.2303	-1.8398	-0.3027	C	0.2303	-1.73	-0.2592
C	-0.7603	2.1206	0.3896	C	-0.7603	2.2304	0.4331
C	0.5535	-3.132	-0.5285	C	0.5535	-3.0222	-0.485
N	1.8579	-3.4824	-0.7515	N	1.8579	-3.3726	-0.708
O	2.1728	-4.741	-0.9715	O	2.1728	-4.6312	-0.928
N	-0.4877	3.0701	-0.5582	N	-1.0788	3.0499	-0.6163
O	-0.8025	4.3288	-0.3381	O	-1.3936	4.3085	-0.3962
O	-0.3085	-3.9782	-0.5337	O	-0.3085	-3.8684	-0.4902
O	-1.2898	2.4381	1.4279	O	-0.7682	2.6627	1.5611
Cl	2.8636	-1.3027	-0.5767	Cl	2.8636	-1.1929	-0.5332
Cl	-3.0704	0.2913	0.4378	Cl	-3.0704	0.4011	0.4813
H	1.677	1.242	-0.059	H	1.677	1.3518	-0.0155

H	-1.8839	-2.2533	-0.0802	H	-1.8839	-2.1435	-0.0367
H	2.5801	-2.7735	-0.7473	H	2.5801	-2.6637	-0.7038
H	3.0704	-4.9821	-1.1249	H	3.0704	-4.8723	-1.0814
H	-0.0441	2.8041	-1.4279	H	-1.0721	2.6876	-1.5611
H	-0.6149	4.9821	-0.9903	H	-1.6127	4.8723	-1.1183
	300°				**330°**		
C	1.2257	-0.6059	-0.3432	C	1.2654	-0.4609	-0.1948
C	0.892	0.7282	-0.1101	C	0.9317	0.8732	0.0383
C	-0.4371	1.0852	0.1172	C	-0.3974	1.2302	0.2656
C	-1.4325	0.1081	0.1112	C	-1.3928	0.2531	0.2596
C	-1.0988	-1.226	-0.122	C	-1.0591	-1.081	0.0264
C	0.2303	-1.583	-0.3492	C	0.27	-1.438	-0.2008
C	-0.7603	2.3774	0.3431	C	-0.7206	2.5224	0.4915
C	0.5535	-2.8752	-0.575	C	0.5932	-2.7302	-0.4266
N	1.8579	-3.2256	-0.798	N	1.8976	-3.0806	-0.6496
O	2.1728	-4.4842	-1.018	O	2.2125	-4.3392	-0.8696
N	-1.6284	3.0227	-0.4961	N	-1.9496	2.9959	0.118
O	-1.9433	4.2814	-0.276	O	-2.2645	4.2546	0.3382
O	-0.3085	-3.7214	-0.5802	O	-0.2688	-3.5764	-0.4318
O	-0.2832	2.9635	1.2856	O	0.0749	3.2599	1.023
Cl	2.8636	-1.0459	-0.6232	Cl	2.9033	-0.9009	-0.4748
Cl	-3.0704	0.5481	0.3913	Cl	-3.0307	0.6931	0.5397
H	1.677	1.4988	-0.1055	H	1.7167	1.6438	0.0429
H	-1.8839	-1.9965	-0.1267	H	-1.8442	-1.8515	0.0217
H	2.5801	-2.5167	-0.7938	H	2.6198	-2.3717	-0.6454
H	3.0704	-4.7253	-1.1714	H	3.1101	-4.5803	-1.023
H	-2.028	2.5317	-1.2856	H	-2.616	2.378	-0.3271
H	-2.5405	4.7253	-0.8535	H	-3.1101	4.5803	0.0811

Table S24 Cartesian coordinates of the H_2-Cl_2-BDHA ligand geometry after co-rotation of both hydroxamate groups.

	0°				**30°**		
C	1.3291	-0.357	-0.2273	C	1.3291	-0.357	-0.2273
C	0.9954	0.9771	0.0058	C	0.9954	0.9771	0.0058
C	-0.3337	1.3341	0.2331	C	-0.3337	1.3341	0.2331
C	-1.3291	0.357	0.2271	C	-1.3291	0.357	0.2271
C	-0.9954	-0.9771	-0.0061	C	-0.9954	-0.9771	-0.0061
C	0.3337	-1.3341	-0.2333	C	0.3337	-1.3341	-0.2333
C	-0.6569	2.6263	0.459	C	-0.6569	2.6263	0.459
C	0.6569	-2.6263	-0.4591	C	0.6569	-2.6263	-0.4591
N	1.9613	-2.9767	-0.6821	N	1.7311	-2.9351	-1.2494
O	2.2762	-4.2353	-0.9021	O	2.046	-4.1937	-1.4695
N	-1.9614	2.9767	0.682	N	-1.7312	2.9351	1.2494

O	-2.2762	4.2354	0.9021	O	-2.046	4.1938	1.4695
O	-0.2051	-3.4725	-0.4643	O	-0.002	-3.5091	0.0363
O	0.2052	3.4725	0.4641	O	0.002	3.5092	-0.0366
Cl	2.967	-0.797	-0.5073	Cl	2.967	-0.797	-0.5073
Cl	-2.967	0.797	0.5072	Cl	-2.967	0.797	0.5072
H	1.7804	1.7477	0.0104	H	1.7804	1.7477	0.0104
H	-1.7805	-1.7476	-0.0108	H	-1.7805	-1.7476	-0.0108
H	2.6835	-2.2678	-0.6779	H	2.2831	-2.1955	-1.6647
H	3.1738	-4.4764	-1.0555	H	2.7852	-4.4062	-2.0133
H	-2.6835	2.2678	0.6777	H	-2.2831	2.1955	1.6645
H	-3.1738	4.4764	1.0555	H	-2.7852	4.4062	2.0133
	60°				**90°**		
C	1.3291	-0.3569	-0.2273	C	1.3291	-0.3569	-0.2273
C	0.9954	0.9772	0.0058	C	0.9954	0.9772	0.0058
C	-0.3337	1.3342	0.2331	C	-0.3337	1.3342	0.2331
C	-1.3291	0.3571	0.2271	C	-1.3291	0.3571	0.2271
C	-0.9954	-0.977	-0.0061	C	-0.9954	-0.977	-0.0061
C	0.3337	-1.334	-0.2333	C	0.3337	-1.334	-0.2333
C	-0.6569	2.6264	0.459	C	-0.6569	2.6264	0.459
C	0.6569	-2.6262	-0.4591	C	0.6569	-2.6262	-0.4591
N	1.257	-2.9862	-1.6357	N	0.6659	-3.1162	-1.7373
O	1.5718	-4.2448	-1.8557	O	0.9807	-4.3749	-1.9574
N	-1.257	2.9862	1.6357	N	-0.6659	3.1163	1.7373
O	-1.5718	4.2449	1.8557	O	-0.9807	4.375	1.9573
O	0.4163	-3.464	0.3771	O	0.9379	-3.3493	0.4668
O	-0.4164	3.4642	-0.3774	O	-0.938	3.3494	-0.467
Cl	2.967	-0.7969	-0.5073	Cl	2.967	-0.7969	-0.5073
Cl	-2.967	0.7971	0.5072	Cl	-2.967	0.7971	0.5072
H	1.7804	1.7478	0.0104	H	1.7804	1.7478	0.0104
H	-1.7805	-1.7475	-0.0108	H	-1.7805	-1.7475	-0.0108
H	1.4584	-2.2843	-2.3364	H	0.4304	-2.5106	-2.5131
H	1.9847	-4.4924	-2.6654	H	0.9869	-4.712	-2.8369
H	-1.4585	2.2843	2.3362	H	-0.4305	2.5106	2.5129
H	-1.9848	4.4924	2.6654	H	-0.9869	4.712	2.8369
	120°				**150°**		
C	1.3291	-0.3569	-0.2273	C	1.3291	-0.357	-0.2274
C	0.9954	0.9772	0.0057	C	0.9954	0.9771	0.0057
C	-0.3337	1.3342	0.233	C	-0.3337	1.3341	0.233
C	-1.3291	0.3571	0.227	C	-1.3291	0.357	0.227
C	-0.9954	-0.977	-0.0061	C	-0.9954	-0.9771	-0.0062
C	0.3337	-1.334	-0.2333	C	0.3337	-1.3341	-0.2334
C	-0.6569	2.6264	0.4589	C	-0.6569	2.6263	0.4589
C	0.6569	-2.6262	-0.4591	C	0.6569	-2.6263	-0.4592
N	0.1163	-3.2904	-1.5271	N	-0.2446	-3.4621	-1.0614
O	0.431	-4.5491	-1.7471	O	0.0701	-4.7208	-1.2813

N	-0.1163	3.2905	1.5271	N	0.2446	3.4622	1.0613
O	-0.4311	4.5492	1.7471	O	-0.0702	4.7209	1.2813
O	1.4228	-3.1956	0.2814	O	1.7413	-3.0441	-0.1296
O	-1.423	3.1957	-0.2815	O	-1.7414	3.0441	0.1295
Cl	2.967	-0.7969	-0.5073	Cl	2.967	-0.797	-0.5074
Cl	-2.967	0.7971	0.5071	Cl	-2.967	0.797	0.5071
H	1.7804	1.7478	0.0103	H	1.7804	1.7477	0.0103
H	-1.7805	-1.7475	-0.0108	H	-1.7805	-1.7476	-0.0109
H	-0.5255	-2.8136	-2.1475	H	-1.1531	-3.1121	-1.3374
H	0.0591	-5.0061	-2.482	H	-0.5502	-5.2959	-1.6958
H	0.5254	2.8135	2.1473	H	1.1531	3.1121	1.3373
H	-0.0591	5.0061	2.482	H	0.5502	5.2959	1.6958
180°				**210°**			
C	1.3291	-0.357	-0.2274	C	1.3291	-0.357	-0.2273
C	0.9954	0.9771	0.0057	C	0.9954	0.9771	0.0058
C	-0.3337	1.3341	0.233	C	-0.3337	1.3341	0.2331
C	-1.3291	0.357	0.227	C	-1.3291	0.357	0.2271
C	-0.9954	-0.9771	-0.0062	C	-0.9954	-0.9771	-0.0061
C	0.3337	-1.3341	-0.2334	C	0.3337	-1.3341	-0.2333
C	-0.6569	2.6263	0.4589	C	-0.6569	2.6263	0.459
C	0.6569	-2.6263	-0.4592	C	0.6569	-2.6263	-0.4591
N	-0.32	-3.5852	-0.465	N	-0.0898	-3.6269	0.1024
O	-0.0053	-4.8439	-0.6848	O	0.2249	-4.8855	-0.1174
N	0.3201	3.5853	0.4648	N	0.0899	3.6269	-0.1025
O	0.0053	4.844	0.6848	O	-0.225	4.8856	0.1175
O	1.8079	-2.9356	-0.6559	O	1.6048	-2.8989	-1.1565
O	-1.808	2.9354	0.6558	O	-1.6048	2.8987	1.1565
Cl	2.967	-0.797	-0.5074	Cl	2.967	-0.797	-0.5073
Cl	-2.967	0.797	0.5071	Cl	-2.967	0.797	0.5072
H	1.7804	1.7477	0.0103	H	1.7804	1.7477	0.0104
H	-1.7805	-1.7476	-0.0109	H	-1.7805	-1.7476	-0.0108
H	-1.2843	-3.3263	-0.3	H	-0.8839	-3.3986	0.6867
H	-0.6776	-5.5038	-0.6889	H	-0.289	-5.574	0.269
H	1.2843	3.3262	0.2999	H	0.8839	3.3986	-0.6868
H	0.6776	5.5038	0.6889	H	0.289	5.574	-0.2689
240°				**270°**			
C	1.3291	-0.3571	-0.2273	C	1.3291	-0.3571	-0.2273
C	0.9954	0.977	0.0058	C	0.9954	0.977	0.0058
C	-0.3337	1.334	0.2331	C	-0.3337	1.334	0.2331
C	-1.3291	0.3569	0.2271	C	-1.3291	0.3569	0.2271
C	-0.9954	-0.9772	-0.0061	C	-0.9954	-0.9772	-0.0061
C	0.3337	-1.3342	-0.2333	C	0.3337	-1.3342	-0.2333
C	-0.6569	2.6262	0.459	C	-0.6569	2.6262	0.459
C	0.6569	-2.6264	-0.4591	C	0.6569	-2.6264	-0.4591
N	0.3843	-3.5758	0.4886	N	0.9754	-3.4457	0.5903

O	0.6991	-4.8344	0.2688	O	1.2902	-4.7044	0.3704
N	-0.3843	3.5758	-0.4888	N	-0.9754	3.4457	-0.5904
O	-0.6991	4.8345	-0.2688	O	-1.2902	4.7044	-0.3704
O	1.1865	-2.944	-1.4973	O	0.6649	-3.0588	-1.587
O	-1.1864	2.9437	1.4973	O	-0.6648	3.0585	1.587
Cl	2.967	-0.7971	-0.5073	Cl	2.967	-0.7971	-0.5073
Cl	-2.967	0.7969	0.5072	Cl	-2.967	0.7969	0.5072
H	1.7804	1.7476	0.0104	H	1.7804	1.7476	0.0104
H	-1.7805	-1.7477	-0.0108	H	-1.7805	-1.7477	-0.0108
H	-0.0592	-3.3097	1.3585	H	0.9688	-3.0835	1.5352
H	0.5115	-5.4877	0.921	H	1.5093	-5.2681	1.0926
H	0.0593	3.3097	-1.3586	H	-0.9687	3.0835	-1.5353
H	-0.5115	5.4877	-0.9209	H	-1.5093	5.2681	-1.0925
300°				**330°**			
C	1.3291	-0.3571	-0.2273	C	1.3291	-0.357	-0.2272
C	0.9954	0.977	0.0058	C	0.9954	0.9771	0.0059
C	-0.3337	1.334	0.2331	C	-0.3337	1.3341	0.2332
C	-1.3291	0.3569	0.2271	C	-1.3291	0.357	0.2272
C	-0.9954	-0.9772	-0.0061	C	-0.9954	-0.9771	-0.006
C	0.3337	-1.3342	-0.2333	C	0.3337	-1.3341	-0.2332
C	-0.6569	2.6262	0.459	C	-0.6569	2.6263	0.4591
C	0.6569	-2.6264	-0.4591	C	0.6569	-2.6263	-0.459
N	1.525	-3.2715	0.3801	N	1.8858	-3.0998	-0.0856
O	1.8399	-4.5301	0.1602	O	2.2008	-4.3584	-0.3055
N	-1.525	3.2715	-0.3802	N	-1.8859	3.0998	0.0856
O	-1.8399	4.5302	-0.1601	O	-2.2008	4.3585	0.3057
O	0.18	-3.2125	-1.4015	O	-0.1385	-3.3639	-0.9905
O	-0.1798	3.2123	1.4015	O	0.1386	3.3638	0.9905
Cl	2.967	-0.7971	-0.5073	Cl	2.967	-0.797	-0.5072
Cl	-2.967	0.7969	0.5072	Cl	-2.967	0.797	0.5073
H	1.7804	1.7476	0.0104	H	1.7804	1.7477	0.0105
H	-1.7805	-1.7477	-0.0108	H	-1.7805	-1.7476	-0.0107
H	1.9247	-2.7805	1.1696	H	2.5523	-2.4819	0.3596
H	2.4372	-4.9741	0.7377	H	3.0464	-4.6843	-0.0485
H	-1.9246	2.7805	-1.1696	H	-2.5523	2.4819	-0.3596
H	-2.4371	4.9741	-0.7376	H	-3.0464	4.6843	0.0487

Table S25 Cartesian coordinates of the H_2-Cl_2-BDHA ligand geometry after counter-rotation of both hydroxamate groups.

0°				**30°**			
C	1.3291	-0.357	-0.2273	C	1.2894	-0.2179	-0.7387
C	0.9954	0.9771	0.0058	C	0.9557	1.1162	-0.5056
C	-0.3337	1.3341	0.2331	C	-0.3734	1.4732	-0.2783

C	-1.3291	0.357	0.2271	C	-1.3688	0.4961	-0.2843
C	-0.9954	-0.9771	-0.0061	C	-1.0352	-0.838	-0.5175
C	0.3337	-1.3341	-0.2333	C	0.294	-1.195	-0.7447
C	-0.6569	2.6263	0.459	C	-0.6966	2.7653	-0.0524
C	0.6569	-2.6263	-0.4591	C	0.6172	-2.4872	-0.9705
N	1.9613	-2.9767	-0.6821	N	1.8462	-2.9607	-0.597
O	2.2762	-4.2353	-0.9021	O	2.161	-4.2194	-0.817
N	-1.9614	2.9767	0.682	N	-1.7708	3.0741	0.738
O	-2.2762	4.2354	0.9021	O	-2.0857	4.3328	0.9581
O	-0.2051	-3.4725	-0.4643	O	-0.1783	-3.2248	-1.502
O	0.2052	3.4725	0.4641	O	-0.0377	3.6483	-0.5479
Cl	2.967	-0.797	-0.5073	Cl	2.9273	-0.658	-1.0187
Cl	-2.967	0.797	0.5072	Cl	-3.0067	0.9361	-0.0042
H	1.7804	1.7477	0.0104	H	1.7407	1.8867	-0.501
H	-1.7805	-1.7476	-0.0108	H	-1.8202	-1.6085	-0.5222
H	2.6835	-2.2678	-0.6779	H	2.5126	-2.3428	-0.1518
H	3.1738	-4.4764	-1.0555	H	3.0067	-4.5453	-0.56
H	-2.6835	2.2678	0.6777	H	-2.3228	2.3344	1.1531
H	-3.1738	4.4764	1.0555	H	-2.8249	4.5453	1.502
	60°				**90°**		
C	1.3291	-0.1162	-0.8593	C	1.3291	-0.0789	-0.8523
C	0.9954	1.2179	-0.6262	C	0.9954	1.2552	-0.6192
C	-0.3337	1.5749	-0.3989	C	-0.3337	1.6122	-0.3919
C	-1.3291	0.5978	-0.4048	C	-1.3291	0.6351	-0.3978
C	-0.9955	-0.7362	-0.638	C	-0.9955	-0.699	-0.631
C	0.3337	-1.0933	-0.8652	C	0.3337	-1.056	-0.8582
C	-0.6569	2.8671	-0.1729	C	-0.6569	2.9044	-0.166
C	0.6569	-2.3854	-1.091	C	0.6569	-2.3482	-1.084
N	1.525	-3.0306	-0.2518	N	0.9754	-3.1676	-0.0346
O	1.8398	-4.2893	-0.4717	O	1.2902	-4.4263	-0.2546
N	-1.257	3.227	1.0037	N	-0.6659	3.3943	1.1123
O	-1.5718	4.4857	1.2238	O	-0.9807	4.653	1.3324
O	0.1799	-2.9715	-2.0335	O	0.6649	-2.7806	-2.212
O	-0.4164	3.705	-1.0093	O	-0.938	3.6274	-1.0919
Cl	2.967	-0.5562	-1.1392	Cl	2.967	-0.5189	-1.1322
Cl	-2.967	1.0379	-0.1247	Cl	-2.967	1.0751	-0.1177
H	1.7804	1.9885	-0.6216	H	1.7804	2.0257	-0.6146
H	-1.7805	-1.5068	-0.6427	H	-1.7805	-1.4695	-0.6357
H	1.9246	-2.5396	0.5377	H	0.9687	-2.8054	0.9103
H	2.4372	-4.7333	0.1057	H	1.5093	-4.9901	0.4676
H	-1.4585	2.525	1.7043	H	-0.4304	2.7885	1.8881
H	-1.9847	4.7333	2.0335	H	-0.9869	4.9901	2.212
	120°				**150°**		
C	1.3291	-0.1162	-0.7197	C	1.3291	-0.218	-0.497
C	0.9954	1.2179	-0.4866	C	0.9954	1.1161	-0.2639

C	-0.3337	1.5749	-0.2593	C	-0.3337	1.4731	-0.0366
C	-1.3291	0.5978	-0.2652	C	-1.3291	0.4961	-0.0425
C	-0.9955	-0.7362	-0.4984	C	-0.9955	-0.838	-0.2757
C	0.3337	-1.0933	-0.7256	C	0.3337	-1.195	-0.5029
C	-0.6569	2.8671	-0.0334	C	-0.6569	2.7653	0.1893
C	0.6569	-2.3855	-0.9514	C	0.6569	-2.4872	-0.7287
N	0.3843	-3.3349	-0.0036	N	-0.0899	-3.4878	-0.1672
O	0.6991	-4.5936	-0.2236	O	0.225	-4.7465	-0.3871
N	-0.1163	3.5313	1.0347	N	0.2446	3.6012	0.7916
O	-0.4311	4.79	1.2548	O	-0.0702	4.8599	1.0117
O	1.1864	-2.703	-1.9897	O	1.6048	-2.7597	-1.4261
O	-1.423	3.4364	-0.7738	O	-1.7414	3.1832	-0.1401
Cl	2.967	-0.5562	-0.9996	Cl	2.967	-0.658	-0.7769
Cl	-2.967	1.0379	0.0149	Cl	-2.967	0.9361	0.2376
H	1.7804	1.9885	-0.482	H	1.7804	1.8867	-0.2593
H	-1.7805	-1.5068	-0.5031	H	-1.7805	-1.6086	-0.2804
H	-0.0594	-3.0689	0.8662	H	-0.884	-3.2595	0.4171
H	0.5115	-5.247	0.4286	H	-0.2889	-5.435	-0.0007
H	0.5255	3.0543	1.655	H	1.1531	3.2511	1.0677
H	-0.0591	5.247	1.9897	H	0.5501	5.435	1.4261
180°				**210°**			
C	1.3291	-0.357	-0.2273	C	1.3291	-0.496	0.0423
C	0.9954	0.9771	0.0058	C	0.9954	0.8381	0.2754
C	-0.3337	1.3341	0.2331	C	-0.3337	1.1951	0.5027
C	-1.3291	0.357	0.2271	C	-1.3291	0.218	0.4968
C	-0.9955	-0.9771	-0.0061	C	-0.9955	-1.1161	0.2636
C	0.3337	-1.3341	-0.2333	C	0.3337	-1.4731	0.0364
C	-0.6569	2.6263	0.459	C	-0.6569	2.4872	0.7286
C	0.6569	-2.6263	-0.4591	C	0.6569	-2.7653	-0.1894
N	-0.3201	-3.5853	-0.4649	N	-0.2446	-3.6012	-0.7917
O	-0.0052	-4.844	-0.6849	O	0.0702	-4.8599	-1.0117
N	0.32	3.5853	0.4648	N	0.0898	3.4879	0.1671
O	0.0052	4.844	0.6849	O	-0.225	4.7466	0.3872
O	1.808	-2.9355	-0.6558	O	1.7414	-3.1831	0.1401
O	-1.808	2.9354	0.6558	O	-1.6048	2.7597	1.4261
Cl	2.967	-0.797	-0.5073	Cl	2.967	-0.9361	-0.2376
Cl	-2.967	0.797	0.5072	Cl	-2.967	0.658	0.7769
H	1.7804	1.7477	0.0104	H	1.7804	1.6086	0.28
H	-1.7805	-1.7476	-0.0108	H	-1.7805	-1.8866	0.2589
H	-1.2844	-3.3262	-0.3001	H	-1.1531	-3.2512	-1.0678
H	-0.6775	-5.5039	-0.6889	H	-0.5501	-5.4351	-1.4261
H	1.2843	3.3263	0.2999	H	0.8839	3.2596	-0.4172
H	0.6774	5.5039	0.6889	H	0.2888	5.4351	0.0008
240°				**270°**			
C	1.3291	-0.5978	0.265	C	1.3291	-0.6351	0.3976

C	0.9954	0.7363	0.4981	C	0.9954	0.699	0.6307
C	-0.3337	1.0933	0.7254	C	-0.3337	1.056	0.858
C	-1.3291	0.1162	0.7195	C	-1.3291	0.079	0.8521
C	-0.9955	-1.2179	0.4863	C	-0.9955	-1.2551	0.6189
C	0.3337	-1.5749	0.2591	C	0.3337	-1.6121	0.3917
C	-0.6569	2.3855	0.9513	C	-0.6569	2.3482	1.084
C	0.6569	-2.8671	0.0333	C	0.6569	-2.9043	0.1659
N	0.1163	-3.5313	-1.0348	N	0.6659	-3.3943	-1.1124
O	0.4311	-4.79	-1.2547	O	0.9808	-4.653	-1.3323
N	-0.3843	3.335	0.0036	N	-0.9754	3.1677	0.0346
O	-0.6992	4.5937	0.2236	O	-1.2903	4.4264	0.2546
O	1.4229	-3.4364	0.7738	O	0.9379	-3.6274	1.0919
O	-1.1864	2.703	1.9897	O	-0.6648	2.7805	2.2119
Cl	2.967	-1.0378	-0.0149	Cl	2.967	-1.0751	0.1177
Cl	-2.967	0.5562	0.9996	Cl	-2.967	0.519	1.1322
H	1.7804	1.5069	0.5027	H	1.7804	1.4696	0.6353
H	-1.7805	-1.9884	0.4816	H	-1.7805	-2.0256	0.6142
H	-0.5254	-3.0544	-1.6551	H	0.4305	-2.7886	-1.8882
H	0.0592	-5.2471	-1.9897	H	0.987	-4.9902	-2.2119
H	0.0592	3.069	-0.8663	H	-0.9688	2.8055	-0.9104
H	-0.5116	5.2471	-0.4285	H	-1.5095	4.9902	-0.4674
300°				**330°**			
C	1.3291	-0.5978	0.4046	C	1.3688	-0.496	0.2841
C	0.9954	0.7363	0.6377	C	1.0351	0.8381	0.5172
C	-0.3337	1.0933	0.865	C	-0.294	1.1951	0.7445
C	-1.3291	0.1162	0.8591	C	-1.2894	0.218	0.7385
C	-0.9955	-1.2179	0.6259	C	-0.9557	-1.1161	0.5053
C	0.3337	-1.5749	0.3987	C	0.3734	-1.4731	0.2781
C	-0.6569	2.3855	1.0909	C	-0.6172	2.4873	0.9704
C	0.6569	-2.8671	0.1729	C	0.6966	-2.7653	0.0523
N	1.257	-3.227	-1.0038	N	1.7709	-3.0741	-0.738
O	1.5719	-4.4857	-1.2237	O	2.0857	-4.3328	-0.958
N	-1.5251	3.0307	0.2518	N	-1.8462	2.9608	0.597
O	-1.8399	4.2894	0.4718	O	-2.1611	4.2195	0.8171
O	0.4163	-3.7049	1.0092	O	0.0377	-3.6482	0.5478
O	-0.1798	2.9715	2.0334	O	0.1783	3.2248	1.5019
Cl	2.967	-1.0378	0.1246	Cl	3.0067	-0.936	0.0041
Cl	-2.967	0.5562	1.1392	Cl	-2.9273	0.658	1.0186
H	1.7804	1.5069	0.6423	H	1.8201	1.6087	0.5218
H	-1.7805	-1.9884	0.6211	H	-1.7408	-1.8866	0.5006
H	1.4585	-2.5251	-1.7044	H	2.3229	-2.3345	-1.1532
H	1.9848	-4.7334	-2.0334	H	2.8249	-4.5453	-1.5019
H	-1.9247	2.5397	-0.5378	H	-2.5126	2.3429	0.1518
H	-2.4373	4.7334	-0.1056	H	-3.0067	4.5453	0.5601

Table S26 Cartesian coordinates of the rotated geometry for the single-side hydroxamate group in the H_2-Br_2-BDHA ligand model.

	0°				30°		
C	0.919	1.0097	0.2852	C	0.942	1.0097	0.266
C	-0.4412	1.3074	0.2042	C	-0.4182	1.3074	0.185
C	-1.3603	0.2976	-0.0812	C	-1.3373	0.2976	-0.1004
C	-0.919	-1.0097	-0.2856	C	-0.896	-1.0097	-0.3047
C	0.4412	-1.3073	-0.2046	C	0.4642	-1.3073	-0.2237
C	1.3603	-0.2976	0.0808	C	1.3833	-0.2976	0.0616
C	-2.6778	0.5859	-0.1596	C	-2.6548	0.5859	-0.1787
C	2.6779	-0.5859	0.1593	C	2.7009	-0.5859	0.1401
N	3.5799	0.4051	0.4395	N	3.6029	0.4051	0.4203
O	4.8633	0.1243	0.5159	O	4.8863	0.1243	0.4967
N	-3.5799	-0.4051	-0.4396	N	-3.5841	-0.3631	0.1529
O	-4.8633	-0.1244	-0.516	O	-4.8675	-0.0824	0.0766
O	3.06	-1.7181	-0.0177	O	3.083	-1.7181	-0.0368
O	-3.06	1.7181	0.0175	O	-3.013	1.6811	-0.5414
Br	2.1584	2.3713	0.6702	Br	2.1814	2.3713	0.651
Br	-2.1584	-2.3713	-0.6704	Br	-2.1354	-2.3713	-0.6895
H	-0.7892	2.3384	0.3653	H	-0.7662	2.3384	0.3461
H	0.7892	-2.3383	-0.3659	H	0.8122	-2.3383	-0.385
H	3.2597	1.3536	0.5878	H	3.2827	1.3536	0.5686
H	5.4839	0.8062	0.7087	H	5.5069	0.8062	0.6895
H	-3.2597	-1.3536	-0.5879	H	-3.2841	-1.2806	0.4568
H	-5.4839	-0.8063	-0.7087	H	-5.5069	-0.7355	0.3048
	60°				**90°**		
C	0.9057	1.0097	0.0889	C	0.82	1.0097	-0.029
C	-0.4545	1.3074	0.0079	C	-0.5402	1.3074	-0.11
C	-1.3736	0.2976	-0.2775	C	-1.4593	0.2976	-0.3954
C	-0.9323	-1.0097	-0.4819	C	-1.018	-1.0097	-0.5998
C	0.4279	-1.3073	-0.4009	C	0.3422	-1.3073	-0.5188
C	1.347	-0.2976	-0.1155	C	1.2613	-0.2976	-0.2334
C	-2.6911	0.5859	-0.3559	C	-2.7768	0.5859	-0.4738
C	2.6646	-0.5859	-0.037	C	2.5789	-0.5859	-0.1549
N	3.5666	0.4051	0.2432	N	3.4809	0.4051	0.1253
O	4.85	0.1243	0.3196	O	4.7643	0.1243	0.2017
N	-3.5774	-0.0277	0.488	N	-3.5616	0.5113	0.6454
O	-4.8608	0.253	0.4117	O	-4.845	0.7921	0.5692
O	3.0467	-1.7181	-0.214	O	2.961	-1.7181	-0.3319
O	-3.0871	1.3852	-1.1704	O	-3.2624	0.9097	-1.5315
Br	2.1451	2.3713	0.4739	Br	2.0594	2.3713	0.356
Br	-2.1717	-2.3713	-0.8667	Br	-2.2574	-2.3713	-0.9846
H	-0.8025	2.3384	0.169	H	-0.8882	2.3384	0.0511
H	0.7759	-2.3383	-0.5622	H	0.6902	-2.3383	-0.6801

H	3.2464	1.3536	0.3915	H	3.1607	1.3536	0.2736
H	5.4706	0.8062	0.5124	H	5.3849	0.8062	0.3945
H	-3.2456	-0.6973	1.1704	H	-3.1548	0.2401	1.5315
H	-5.4706	-0.1692	0.9923	H	-5.3849	0.7406	1.3393
120°				**150°**			
C	0.7078	1.0097	-0.0139	C	0.5991	0.9006	0.1301
C	-0.6524	1.3074	-0.0949	C	-0.7611	1.1983	0.0491
C	-1.5715	0.2976	-0.3803	C	-1.6802	0.1885	-0.2363
C	-1.1302	-1.0097	-0.5847	C	-1.2389	-1.1188	-0.4407
C	0.23	-1.3073	-0.5037	C	0.1213	-1.4164	-0.3597
C	1.1491	-0.2976	-0.2183	C	1.0404	-0.4067	-0.0743
C	-2.889	0.5859	-0.4587	C	-2.9977	0.4768	-0.3147
C	2.4667	-0.5859	-0.1398	C	2.358	-0.695	0.0042
N	3.3687	0.4051	0.1404	N	3.26	0.296	0.2844
O	4.6521	0.1243	0.2168	O	4.5434	0.0152	0.3608
N	-3.5409	1.1094	0.6254	N	-3.5208	1.4973	0.4332
O	-4.8243	1.3902	0.5491	O	-4.8042	1.7782	0.3569
O	2.8488	-1.7181	-0.3168	O	2.7401	-1.8272	-0.1728
O	-3.492	0.382	-1.4855	O	-3.7143	-0.1657	-1.0448
Br	1.9472	2.3713	0.3711	Br	1.8385	2.2622	0.5151
Br	-2.3696	-2.3713	-0.9695	Br	-2.4783	-2.4804	-0.8255
H	-1.0004	2.3384	0.0662	H	-1.1091	2.2293	0.2102
H	0.578	-2.3383	-0.665	H	0.4693	-2.4474	-0.521
H	3.0485	1.3536	0.2887	H	2.9398	1.2445	0.4327
H	5.2727	0.8062	0.4096	H	5.164	0.6971	0.5536
H	-3.0357	1.2803	1.4855	H	-2.9205	2.0356	1.0448
H	-5.2727	1.7504	1.2951	H	-5.164	2.4804	0.8715
180°				**210°**			
C	0.5231	0.6789	0.266	C	0.5001	0.7143	0.3958
C	-0.8371	0.9766	0.185	C	-0.8601	1.012	0.3148
C	-1.7562	-0.0332	-0.1004	C	-1.7792	0.0022	0.0294
C	-1.3149	-1.3405	-0.3048	C	-1.3379	-1.3051	-0.175
C	0.0453	-1.6381	-0.2238	C	0.0223	-1.6027	-0.094
C	0.9644	-0.6284	0.0616	C	0.9414	-0.593	0.1914
C	-3.0737	0.2551	-0.1788	C	-3.0967	0.2905	-0.049
C	2.282	-0.9167	0.1401	C	2.259	-0.8813	0.2699
N	3.184	0.0743	0.4203	N	3.161	0.1097	0.5501
O	4.4674	-0.2065	0.4967	O	4.4444	-0.1711	0.6265
N	-3.5068	1.5383	0.0218	N	-3.5025	1.5317	-0.4601
O	-4.7901	1.8192	-0.0545	O	-4.7859	1.8127	-0.5365
O	2.6641	-2.0489	-0.0369	O	2.6411	-2.0135	0.0929
O	-3.8697	-0.6193	-0.426	O	-3.9167	-0.5469	0.2435
Br	1.7625	2.0405	0.651	Br	1.7395	2.0759	0.7808
Br	-2.5543	-2.7021	-0.6895	Br	-2.5773	-2.6667	-0.5598
H	-1.1851	2.0076	0.3461	H	-1.2081	2.043	0.4759

H	0.3933	-2.6691	-0.3851	H	0.3703	-2.6337	-0.2553
H	2.8638	1.0228	0.5686	H	2.8408	1.0582	0.6984
H	5.088	0.4754	0.6895	H	5.065	0.5108	0.8193
H	-2.8399	2.2708	0.2288	H	-2.8155	2.2332	-0.7052
H	-5.088	2.7021	0.0835	H	-5.065	2.6667	-0.8193
	240°				**270°**		
C	0.5363	0.9974	0.8282	C	0.6221	1.0097	1.001
C	-0.8239	1.2951	0.7472	C	-0.7381	1.3074	0.92
C	-1.743	0.2853	0.4618	C	-1.6572	0.2976	0.6346
C	-1.3017	-1.022	0.2574	C	-1.2159	-1.0097	0.4302
C	0.0585	-1.3196	0.3384	C	0.1443	-1.3073	0.5112
C	0.9776	-0.3099	0.6238	C	1.0634	-0.2976	0.7966
C	-3.0605	0.5736	0.3834	C	-2.9747	0.5859	0.5562
C	2.2952	-0.5982	0.7023	C	2.381	-0.5859	0.8751
N	3.1972	0.3928	0.9825	N	3.283	0.4051	1.1553
O	4.4806	0.112	1.0589	O	4.5664	0.1243	1.2317
N	-3.5092	1.4794	-0.5399	N	-3.5251	0.9527	-0.6425
O	-4.7926	1.7603	-0.6164	O	-4.8084	1.2336	-0.719
O	2.6773	-1.7304	0.5253	O	2.7631	-1.7181	0.6981
O	-3.8427	0.0321	1.1278	O	-3.6674	0.5199	1.5438
Br	1.7757	2.359	1.2132	Br	1.8615	2.3713	1.386
Br	-2.5411	-2.3836	-0.1274	Br	-2.4553	-2.3713	0.0454
H	-1.1719	2.3261	0.9083	H	-1.0861	2.3384	1.0811
H	0.4065	-2.3506	0.1771	H	0.4923	-2.3383	0.3499
H	2.877	1.3413	1.1308	H	2.9628	1.3536	1.3036
H	5.1012	0.7939	1.2517	H	5.187	0.8062	1.4245
H	-2.8539	1.933	-1.1636	H	-2.9448	1.0079	-1.4698
H	-5.1012	2.3836	-1.2517	H	-5.187	1.486	-1.5438
	300°				**330°**		
C	0.7343	1.0097	0.9868	C	0.843	1.0097	0.7472
C	-0.6259	1.3074	0.9058	C	-0.5172	1.3074	0.6662
C	-1.545	0.2976	0.6204	C	-1.4363	0.2976	0.3808
C	-1.1037	-1.0097	0.416	C	-0.995	-1.0097	0.1764
C	0.2565	-1.3073	0.497	C	0.3652	-1.3073	0.2574
C	1.1756	-0.2976	0.7824	C	1.2843	-0.2976	0.5428
C	-2.8625	0.5859	0.542	C	-2.7538	0.5859	0.3024
C	2.4932	-0.5859	0.8609	C	2.6019	-0.5859	0.6213
N	3.3952	0.4051	1.1411	N	3.5039	0.4051	0.9015
O	4.6786	0.1243	1.2175	O	4.7873	0.1243	0.9779
N	-3.5458	0.3546	-0.6215	N	-3.5659	-0.1424	-0.5249
O	-4.8292	0.6354	-0.698	O	-4.8493	0.1383	-0.6014
O	2.8753	-1.7181	0.6839	O	2.984	-1.7181	0.4443
O	-3.4378	1.0477	1.4987	O	-3.2155	1.4862	0.9623
Br	1.9737	2.3713	1.3718	Br	2.0824	2.3713	1.1322
Br	-2.3431	-2.3713	0.0312	Br	-2.2344	-2.3713	-0.2084

H	-0.9739	2.3384	1.0669	H	-0.8652	2.3384	0.8273
H	0.6045	-2.3383	0.3357	H	0.7132	-2.3383	0.0961
H	3.075	1.3536	1.2894	H	3.1837	1.3536	1.0498
H	5.2992	0.8062	1.4103	H	5.4079	0.8062	1.1707
H	-3.0638	-0.0323	-1.4229	H	-3.1791	-0.8967	-1.0778
H	-5.2992	0.4762	-1.4987	H	-5.4079	-0.3628	-1.1707

Table S27 Cartesian coordinates of the H_2-Cl_2-BDHA ligand geometry after co-rotation of both hydroxamate groups.

0°				**30°**			
C	0.919	1.0097	0.2852	C	0.919	1.0097	0.2853
C	-0.4412	1.3074	0.2042	C	-0.4412	1.3074	0.2043
C	-1.3603	0.2976	-0.0812	C	-1.3603	0.2976	-0.0811
C	-0.919	-1.0097	-0.2856	C	-0.919	-1.0097	-0.2855
C	0.4412	-1.3073	-0.2046	C	0.4412	-1.3073	-0.2045
C	1.3603	-0.2976	0.0808	C	1.3603	-0.2976	0.0809
C	-2.6778	0.5859	-0.1596	C	-2.6778	0.5859	-0.1595
C	2.6779	-0.5859	0.1593	C	2.6779	-0.5859	0.1594
N	3.5799	0.4051	0.4395	N	3.6071	0.3632	-0.1721
O	4.8633	0.1243	0.5159	O	4.8905	0.0824	-0.0957
N	-3.5799	-0.4051	-0.4396	N	-3.6072	-0.3631	0.1722
O	-4.8633	-0.1244	-0.516	O	-4.8906	-0.0824	0.0958
O	3.06	-1.7181	-0.0177	O	3.0359	-1.6811	0.5221
O	-3.06	1.7181	0.0175	O	-3.036	1.6811	-0.5221
Br	2.1584	2.3713	0.6702	Br	2.1584	2.3713	0.6703
Br	-2.1584	-2.3713	-0.6704	Br	-2.1584	-2.3713	-0.6703
H	-0.7892	2.3384	0.3653	H	-0.7892	2.3384	0.3654
H	0.7892	-2.3383	-0.3659	H	0.7892	-2.3383	-0.3658
H	3.2597	1.3536	0.5878	H	3.3071	1.2807	-0.4759
H	5.4839	0.8062	0.7087	H	5.5299	0.7354	-0.3238
H	-3.2597	-1.3536	-0.5879	H	-3.3071	-1.2806	0.476
H	-5.4839	-0.8063	-0.7087	H	-5.5299	-0.7355	0.324
60°				**90°**			
C	0.9189	1.0097	0.2853	C	0.9189	1.0097	0.2853
C	-0.4413	1.3074	0.2043	C	-0.4413	1.3074	0.2043
C	-1.3604	0.2976	-0.0811	C	-1.3604	0.2976	-0.0811
C	-0.9191	-1.0097	-0.2855	C	-0.9191	-1.0097	-0.2855
C	0.4411	-1.3073	-0.2045	C	0.4411	-1.3073	-0.2045
C	1.3602	-0.2976	0.0809	C	1.3602	-0.2976	0.0809
C	-2.6779	0.5859	-0.1595	C	-2.6779	0.5859	-0.1595
C	2.6778	-0.5859	0.1594	C	2.6778	-0.5859	0.1594
N	3.5642	0.0278	-0.6843	N	3.4627	-0.5111	-0.9597
O	4.8476	-0.253	-0.6079	O	4.7461	-0.792	-0.8833

N	-3.5643	-0.0277	0.6843	N	-3.4628	0.5113	0.9598
O	-4.8477	0.253	0.6081	O	-4.7462	0.7921	0.8835
O	3.0737	-1.3852	0.9741	O	3.1632	-0.9096	1.2171
O	-3.0739	1.3852	-0.9741	O	-3.1635	0.9097	-1.2171
Br	2.1583	2.3713	0.6703	Br	2.1583	2.3713	0.6703
Br	-2.1585	-2.3713	-0.6703	Br	-2.1585	-2.3713	-0.6703
H	-0.7893	2.3384	0.3654	H	-0.7893	2.3384	0.3654
H	0.7891	-2.3383	-0.3658	H	0.7891	-2.3383	-0.3658
H	3.2325	0.6974	-1.3668	H	3.0559	-0.2399	-1.8458
H	5.4575	0.1693	-1.1884	H	5.2861	-0.7405	-1.6534
H	-3.2325	-0.6973	1.3668	H	-3.0559	0.2401	1.8458
H	-5.4575	-0.1692	1.1887	H	-5.2861	0.7406	1.6537
120°				**150°**			
C	0.9189	1.0097	0.2854	C	0.9189	1.0096	0.2854
C	-0.4413	1.3074	0.2044	C	-0.4413	1.3073	0.2044
C	-1.3604	0.2976	-0.081	C	-1.3604	0.2975	-0.081
C	-0.9191	-1.0097	-0.2854	C	-0.9191	-1.0098	-0.2854
C	0.4411	-1.3073	-0.2044	C	0.4411	-1.3074	-0.2044
C	1.3602	-0.2976	0.081	C	1.3602	-0.2977	0.081
C	-2.6779	0.5859	-0.1594	C	-2.6779	0.5858	-0.1594
C	2.6778	-0.5859	0.1595	C	2.6778	-0.586	0.1595
N	3.3297	-1.1092	-0.9246	N	3.2009	-1.6064	-0.5884
O	4.6131	-1.3901	-0.8482	O	4.4843	-1.8872	-0.5119
N	-3.3298	1.1094	0.9247	N	-3.201	1.6063	0.5885
O	-4.6132	1.3902	0.8485	O	-4.4844	1.8872	0.5122
O	3.2805	-0.3818	1.1862	O	3.3942	0.0566	0.8896
O	-3.2809	0.382	-1.1862	O	-3.3945	-0.0567	-0.8895
Br	2.1583	2.3713	0.6704	Br	2.1583	2.3712	0.6704
Br	-2.1585	-2.3713	-0.6702	Br	-2.1585	-2.3714	-0.6702
H	-0.7893	2.3384	0.3655	H	-0.7893	2.3383	0.3655
H	0.7891	-2.3383	-0.3657	H	0.7891	-2.3384	-0.3657
H	2.8246	-1.2801	-1.7848	H	2.6007	-2.1447	-1.2
H	5.0616	-1.7502	-1.5941	H	4.8442	-2.5893	-1.0265
H	-2.8247	1.2803	1.7848	H	-2.6007	2.1445	1.2
H	-5.0616	1.7504	1.5944	H	-4.8442	2.5893	1.0268
180°				**210°**			
C	0.9189	1.0096	0.2853	C	0.9189	1.0096	0.2854
C	-0.4413	1.3073	0.2043	C	-0.4413	1.3073	0.2044
C	-1.3604	0.2975	-0.0811	C	-1.3604	0.2975	-0.081
C	-0.9191	-1.0098	-0.2855	C	-0.9191	-1.0098	-0.2854
C	0.4411	-1.3074	-0.2045	C	0.4411	-1.3074	-0.2044
C	1.3602	-0.2977	0.0809	C	1.3602	-0.2977	0.081
C	-2.6779	0.5858	-0.1595	C	-2.6779	0.5858	-0.1594
C	2.6778	-0.586	0.1594	C	2.6778	-0.586	0.1595
N	3.1109	-1.8691	-0.0413	N	3.0836	-1.8272	0.5705

O	4.3942	-2.1499	0.0353	O	4.367	-2.108	0.647
N	-3.111	1.869	0.041	N	-3.0837	1.827	-0.5706
O	-4.3943	2.1499	-0.0353	O	-4.367	2.108	-0.647
O	3.4737	0.2885	0.4066	O	3.4978	0.2515	-0.1331
O	-3.4739	-0.2886	-0.4067	O	-3.4979	-0.2516	0.1331
Br	2.1583	2.3712	0.6703	Br	2.1583	2.3712	0.6704
Br	-2.1585	-2.3714	-0.6703	Br	-2.1585	-2.3714	-0.6702
H	-0.7893	2.3383	0.3654	H	-0.7893	2.3383	0.3655
H	0.7891	-2.3384	-0.3658	H	0.7891	-2.3384	-0.3657
H	2.444	-2.6016	-0.2484	H	2.3966	-2.5287	0.8155
H	4.6922	-3.0328	-0.1028	H	4.6462	-2.962	0.9298
H	-2.4441	2.6015	0.2481	H	-2.3967	2.5285	-0.8157
H	-4.6922	3.0328	0.1028	H	-4.6462	2.962	-0.9298
240°				**270°**			
C	0.919	1.0097	0.2854	C	0.919	1.0097	0.2853
C	-0.4412	1.3074	0.2044	C	-0.4412	1.3074	0.2043
C	-1.3603	0.2976	-0.081	C	-1.3603	0.2976	-0.0811
C	-0.919	-1.0097	-0.2854	C	-0.919	-1.0097	-0.2855
C	0.4412	-1.3073	-0.2044	C	0.4412	-1.3073	-0.2045
C	1.3603	-0.2976	0.081	C	1.3603	-0.2976	0.0809
C	-2.6778	0.5859	-0.1594	C	-2.6778	0.5859	-0.1595
C	2.6779	-0.5859	0.1595	C	2.6779	-0.5859	0.1594
N	3.1265	-1.4918	1.0827	N	3.2281	-0.9528	1.3582
O	4.4099	-1.7725	1.1592	O	4.5115	-1.2336	1.4346
N	-3.1266	1.4917	-1.0827	N	-3.2281	0.9527	-1.3582
O	-4.4099	1.7726	-1.1592	O	-4.5114	1.2336	-1.4347
O	3.46	-0.0444	-0.585	O	3.3705	-0.52	-0.8281
O	-3.46	0.0444	0.585	O	-3.3704	0.5199	0.8281
Br	2.1584	2.3713	0.6704	Br	2.1584	2.3713	0.6703
Br	-2.1584	-2.3713	-0.6702	Br	-2.1584	-2.3713	-0.6703
H	-0.7892	2.3384	0.3655	H	-0.7892	2.3384	0.3654
H	0.7892	-2.3383	-0.3657	H	0.7892	-2.3383	-0.3658
H	2.4712	-1.9454	1.7063	H	2.6478	-1.0081	2.1854
H	4.7186	-2.3958	1.7944	H	4.89	-1.486	2.2594
H	-2.4713	1.9452	-1.7064	H	-2.6478	1.0079	-2.1855
H	-4.7186	2.3958	-1.7944	H	-4.89	1.486	-2.2594
300°				**330°**			
C	0.919	1.0097	0.2853	C	0.919	1.0097	0.2852
C	-0.4412	1.3074	0.2043	C	-0.4412	1.3074	0.2042
C	-1.3603	0.2976	-0.0811	C	-1.3603	0.2976	-0.0812
C	-0.919	-1.0097	-0.2855	C	-0.919	-1.0097	-0.2856
C	0.4412	-1.3073	-0.2045	C	0.4412	-1.3073	-0.2046
C	1.3603	-0.2976	0.0809	C	1.3603	-0.2976	0.0808
C	-2.6778	0.5859	-0.1595	C	-2.6778	0.5859	-0.1596
C	2.6779	-0.5859	0.1594	C	2.6779	-0.5859	0.1593

N	3.3611	-0.3547	1.3231	N	3.4898	0.1423	0.9868
O	4.6445	-0.6354	1.3995	O	4.7732	-0.1384	1.0632
N	-3.361	0.3546	-1.3231	N	-3.4898	-0.1424	-0.9868
O	-4.6444	0.6354	-1.3996	O	-4.7732	0.1383	-1.0633
O	3.2532	-1.0477	-0.7972	O	3.1395	-1.4863	-0.5005
O	-3.2531	1.0477	0.7971	O	-3.1394	1.4862	0.5004
Br	2.1584	2.3713	0.6703	Br	2.1584	2.3713	0.6702
Br	-2.1584	-2.3713	-0.6703	Br	-2.1584	-2.3713	-0.6704
H	-0.7892	2.3384	0.3654	H	-0.7892	2.3384	0.3653
H	0.7892	-2.3383	-0.3658	H	0.7892	-2.3383	-0.3659
H	2.8791	0.0322	2.1244	H	3.103	0.8966	1.5396
H	5.1145	-0.4764	2.2002	H	5.3318	0.3627	1.6326
H	-2.8791	-0.0323	-2.1244	H	-3.103	-0.8967	-1.5397
H	-5.1145	0.4762	-2.2002	H	-5.3318	-0.3628	-1.6326

Table S28 Cartesian coordinates of the H_2-Br_2-BDHA ligand geometry after counter-rotation of both hydroxamate groups.

0°				**30°**			
C	0.919	1.0097	0.2852	C	1.018	1.0097	-0.1958
C	-0.4412	1.3074	0.2042	C	-0.3422	1.3074	-0.2768
C	-1.3603	0.2976	-0.0812	C	-1.2613	0.2976	-0.5622
C	-0.919	-1.0097	-0.2856	C	-0.82	-1.0097	-0.7666
C	0.4412	-1.3073	-0.2046	C	0.5402	-1.3073	-0.6857
C	1.3603	-0.2976	0.0808	C	1.4593	-0.2976	-0.4002
C	-2.6778	0.5859	-0.1596	C	-2.5788	0.5859	-0.6406
C	2.6779	-0.5859	0.1593	C	2.7769	-0.5859	-0.3217
N	3.5799	0.4051	0.4395	N	3.5888	0.1424	0.5057
O	4.8633	0.1243	0.5159	O	4.8722	-0.1384	0.5821
N	-3.5799	-0.4051	-0.4396	N	-3.5081	-0.3632	-0.309
O	-4.8633	-0.1244	-0.516	O	-4.7915	-0.0824	-0.3854
O	3.06	-1.7181	-0.0177	O	3.2385	-1.4862	-0.9817
O	-3.06	1.7181	0.0175	O	-2.937	1.6811	-1.0033
Br	2.1584	2.3713	0.6702	Br	2.2574	2.3713	0.1892
Br	-2.1584	-2.3713	-0.6704	Br	-2.0594	-2.3713	-1.1515
H	-0.7892	2.3384	0.3653	H	-0.6902	2.3384	-0.1157
H	0.7892	-2.3383	-0.3659	H	0.8882	-2.3383	-0.847
H	3.2597	1.3536	0.5878	H	3.202	0.8966	1.0585
H	5.4839	0.8062	0.7087	H	5.4309	0.3626	1.1515
H	-3.2597	-1.3536	-0.5879	H	-3.208	-1.2807	-0.0052
H	-5.4839	-0.8063	-0.7087	H	-5.4309	-0.7355	-0.1572
60°				**90°**			
C	1.0905	1.0097	-0.3277	C	1.1171	1.0097	-0.2358
C	-0.2697	1.3074	-0.4087	C	-0.2432	1.3074	-0.3168

C	-1.1888	0.2976	-0.6941	C	-1.1623	0.2976	-0.6022
C	-0.7475	-1.0097	-0.8985	C	-0.721	-1.0097	-0.8066
C	0.6127	-1.3073	-0.8176	C	0.6393	-1.3073	-0.7256
C	1.5318	-0.2976	-0.5321	C	1.5583	-0.2976	-0.4402
C	-2.5063	0.5859	-0.7725	C	-2.4798	0.5859	-0.6806
C	2.8493	-0.5859	-0.4536	C	2.8759	-0.5859	-0.3617
N	3.5325	-0.3547	0.71	N	3.4261	-0.9528	0.837
O	4.8159	-0.6355	0.7864	O	4.7095	-1.2336	0.9134
N	-3.3927	-0.0278	0.0713	N	-3.2646	0.5111	0.4387
O	-4.6761	0.253	-0.0051	O	-4.5481	0.7919	0.3623
O	3.4246	-1.0477	-1.4102	O	3.5685	-0.5199	-1.3492
O	-2.9024	1.3851	-1.5871	O	-2.9654	0.9096	-1.7382
Br	2.3299	2.3713	0.0573	Br	2.3564	2.3713	0.1492
Br	-1.9869	-2.3713	-1.2834	Br	-1.9604	-2.3713	-1.1914
H	-0.6177	2.3384	-0.2476	H	-0.5912	2.3384	-0.1557
H	0.9607	-2.3383	-0.9788	H	0.9872	-2.3383	-0.8869
H	3.0506	0.0322	1.5114	H	2.8459	-1.008	1.6643
H	5.286	-0.4764	1.5871	H	5.0881	-1.486	1.7382
H	-3.0609	-0.6974	0.7537	H	-2.8578	0.2399	1.3247
H	-5.286	-0.1693	0.5755	H	-5.0881	0.7405	1.1324
120°				**150°**			
C	1.0905	1.0219	-0.0187	C	1.018	1.1961	0.1301
C	-0.2697	1.3196	-0.0998	C	-0.3422	1.4938	0.049
C	-1.1888	0.3099	-0.3851	C	-1.2613	0.484	-0.2363
C	-0.7475	-0.9974	-0.5896	C	-0.82	-0.8233	-0.4408
C	0.6127	-1.2951	-0.5086	C	0.5402	-1.1209	-0.3598
C	1.5318	-0.2853	-0.2232	C	1.4593	-0.1112	-0.0744
C	-2.5063	0.5981	-0.4635	C	-2.5788	0.7723	-0.3147
C	2.8493	-0.5736	-0.1447	C	2.7769	-0.3995	0.0041
N	3.298	-1.4794	0.7785	N	3.1827	-1.6407	0.4152
O	4.5815	-1.7602	0.855	O	4.4661	-1.9215	0.4916
N	-3.1582	1.1215	0.6206	N	-3.102	1.7926	0.4332
O	-4.4417	1.4023	0.5442	O	-4.3854	2.0734	0.3568
O	3.6315	-0.0321	-0.8891	O	3.5969	0.438	-0.2884
O	-3.1092	0.3941	-1.4902	O	-3.2953	0.1296	-1.0448
Br	2.3299	2.3835	0.3662	Br	2.2574	2.5576	0.515
Br	-1.9869	-2.359	-0.9744	Br	-2.0594	-2.1849	-0.8256
H	-0.6177	2.3506	0.0614	H	-0.6902	2.5248	0.2102
H	0.9607	-2.326	-0.6699	H	0.8882	-2.1519	-0.5211
H	2.6428	-1.9331	1.4022	H	2.4958	-2.3422	0.6602
H	4.8902	-2.3835	1.4902	H	4.7454	-2.7755	0.7744
H	-2.6532	1.2924	1.4807	H	-2.5017	2.331	1.0448
H	-4.8902	1.7624	1.2902	H	-4.7454	2.7755	0.8714
180°				**210°**			
C	0.919	1.0097	0.2853	C	0.82	0.8233	0.4407

C	-0.4412	1.3074	0.2043	C	-0.5402	1.121	0.3596
C	-1.3603	0.2976	-0.0811	C	-1.4593	0.1113	0.0742
C	-0.919	-1.0096	-0.2855	C	-1.018	-1.196	-0.1302
C	0.4412	-1.3073	-0.2045	C	0.3422	-1.4937	-0.0492
C	1.3603	-0.2976	0.0809	C	1.2613	-0.484	0.2362
C	-2.6778	0.5859	-0.1594	C	-2.7768	0.3995	-0.0041
C	2.6779	-0.5859	0.1594	C	2.5788	-0.7722	0.3147
N	3.111	-1.869	-0.0412	N	3.102	-1.7926	-0.4332
O	4.3944	-2.1498	0.0352	O	4.3854	-2.0734	-0.3567
N	-3.1109	1.869	0.0412	N	-3.1827	1.6407	-0.4152
O	-4.3944	2.1498	-0.0352	O	-4.4662	1.9214	-0.4915
O	3.4738	0.2886	0.4066	O	3.2953	-0.1296	1.0448
O	-3.4738	-0.2886	-0.4066	O	-3.5968	-0.4379	0.2885
Br	2.1584	2.3713	0.6703	Br	2.0594	2.1849	0.8256
Br	-2.1584	-2.3712	-0.6703	Br	-2.2574	-2.5576	-0.515
H	-0.7892	2.3384	0.3654	H	-0.8882	2.152	0.5207
H	0.7892	-2.3383	-0.3658	H	0.6902	-2.5247	-0.2105
H	2.4442	-2.6015	-0.2483	H	2.5018	-2.3309	-1.0448
H	4.6924	-3.0326	-0.1028	H	4.7454	-2.7755	-0.8713
H	-2.4441	2.6016	0.2482	H	-2.4958	2.3422	-0.6603
H	-4.6924	3.0326	0.1029	H	-4.7454	2.7755	-0.7744
240°				**270°**			
C	0.7475	0.9974	0.5894	C	0.721	1.0097	0.8064
C	-0.6127	1.2951	0.5084	C	-0.6392	1.3074	0.7254
C	-1.5318	0.2854	0.223	C	-1.5583	0.2976	0.44
C	-1.0905	-1.0219	0.0186	C	-1.117	-1.0097	0.2356
C	0.2697	-1.3196	0.0995	C	0.2432	-1.3073	0.3165
C	1.1888	-0.3098	0.385	C	1.1623	-0.2976	0.602
C	-2.8493	0.5736	0.1446	C	-2.8759	0.5859	0.3616
C	2.5064	-0.5981	0.4635	C	2.4798	-0.5859	0.6805
N	3.1583	-1.1214	-0.6206	N	3.2647	-0.5111	-0.4387
O	4.4417	-1.4022	-0.5442	O	4.5482	-0.7919	-0.3622
N	-3.2981	1.4794	-0.7786	N	-3.4262	0.9527	-0.837
O	-4.5815	1.7602	-0.855	O	-4.7096	1.2335	-0.9134
O	3.1092	-0.3941	1.4902	O	2.9653	-0.9096	1.7382
O	-3.6314	0.0321	0.8891	O	-3.5684	0.5199	1.3492
Br	1.9869	2.359	0.9744	Br	1.9604	2.3713	1.1914
Br	-2.3299	-2.3835	-0.3663	Br	-2.3564	-2.3713	-0.1493
H	-0.9607	2.3261	0.6695	H	-0.9872	2.3384	0.8865
H	0.6177	-2.3505	-0.0618	H	0.5912	-2.3383	0.1553
H	2.6533	-1.2924	-1.4808	H	2.858	-0.2399	-1.3248
H	4.8903	-1.7623	-1.2901	H	5.0882	-0.7405	-1.1323
H	-2.6429	1.9331	-1.4023	H	-2.846	1.008	-1.6644
H	-4.8903	2.3835	-1.4902	H	-5.0882	1.4859	-1.7382
300°				**330°**			

C	0.7475	1.0097	0.8983	C	0.82	1.0097	0.7664
C	-0.6127	1.3074	0.8173	C	-0.5402	1.3074	0.6854
C	-1.5318	0.2976	0.5319	C	-1.4593	0.2976	0.4
C	-1.0905	-1.0097	0.3275	C	-1.018	-1.0097	0.1956
C	0.2697	-1.3073	0.4084	C	0.3422	-1.3073	0.2765
C	1.1888	-0.2976	0.6939	C	1.2613	-0.2976	0.562
C	-2.8493	0.5859	0.4535	C	-2.7768	0.5859	0.3216
C	2.5064	-0.5859	0.7724	C	2.5788	-0.5859	0.6405
N	3.3928	0.0278	-0.0713	N	3.5081	0.3632	0.309
O	4.6762	-0.253	0.0051	O	4.7915	0.0824	0.3854
N	-3.5326	0.3546	-0.71	N	-3.5888	-0.1424	-0.5057
O	-4.816	0.6354	-0.7864	O	-4.8722	0.1384	-0.5821
O	2.9023	-1.3852	1.587	O	2.937	-1.6811	1.0031
O	-3.4245	1.0477	1.4102	O	-3.2385	1.4862	0.9815
Br	1.9869	2.3713	1.2833	Br	2.0594	2.3713	1.1514
Br	-2.3299	-2.3713	-0.0573	Br	-2.2574	-2.3713	-0.1893
H	-0.9607	2.3384	0.9784	H	-0.8882	2.3384	0.8465
H	0.6177	-2.3383	0.2472	H	0.6902	-2.3383	0.1152
H	3.0611	0.6974	-0.7538	H	3.2081	1.2807	0.0051
H	5.2861	0.1693	-0.5754	H	5.431	0.7354	0.1573
H	-3.0507	-0.0323	-1.5114	H	-3.2021	-0.8967	-1.0586
H	-5.2861	0.4763	-1.587	H	-5.431	-0.3627	-1.1514

Table S29 Cartesian coordinates of the rotated geometry for the single-side hydroxamate group in the PZDH ligand model.

0°				**30°**			
N	1.3343	0.4674	-0.1073	N	1.501	0.4608	0.3386
C	1.0298	-0.8491	-0.0452	C	1.1965	-0.8557	0.4007
C	-0.2737	-1.3058	0.0598	C	-0.107	-1.3124	0.5057
N	-1.3342	-0.4674	0.1074	N	-1.1675	-0.474	0.5533
C	-1.0298	0.8492	0.0453	C	-0.8631	0.8426	0.4912
C	0.2737	1.3058	-0.0597	C	0.4404	1.2992	0.3862
C	-0.494	-2.6375	0.1168	C	-0.3273	-2.6441	0.5627
C	0.494	2.6375	-0.1167	C	0.6607	2.6309	0.3292
N	1.7725	3.116	-0.2208	N	1.7417	3.1172	-0.3558
O	1.9871	4.4132	-0.2764	O	1.9562	4.4144	-0.4114
N	-1.7725	-3.1159	0.2207	N	-1.6058	-3.1225	0.6667
O	-1.987	-4.4131	0.2763	O	-1.8204	-4.4197	0.7222
O	-0.437	3.406	-0.076	O	-0.0961	3.3925	0.8826
O	0.4371	-3.406	0.0759	O	0.6038	-3.4126	0.5219
H	1.8475	-1.5841	-0.0794	H	2.0142	-1.5907	0.3665
H	-1.8475	1.5842	0.0794	H	-1.6808	1.5776	0.5253
H	2.5525	2.4722	-0.2548	H	2.3758	2.4792	-0.8193
H	2.8668	4.7424	-0.3478	H	2.7001	4.749	-0.8826

H	-2.5524	-2.4721	0.2548	H	-2.3858	-2.4787	0.7008
H	-2.8668	-4.7424	0.3478	H	-2.7001	-4.749	0.7938
60°				**90°**			
N	1.844	0.4116	0.5019	N	1.844	0.333	0.5506
C	1.5395	-0.9049	0.564	C	1.5395	-0.9835	0.6127
C	0.236	-1.3616	0.669	C	0.236	-1.4402	0.7177
N	-0.8245	-0.5232	0.7166	N	-0.8245	-0.6018	0.7653
C	-0.5201	0.7934	0.6545	C	-0.5201	0.7148	0.7032
C	0.7834	1.25	0.5495	C	0.7834	1.1714	0.5982
C	0.0157	-2.6933	0.726	C	0.0157	-2.7719	0.7747
C	1.0037	2.5817	0.4925	C	1.0037	2.5031	0.5412
N	1.6274	3.1263	-0.5978	N	1.0329	3.1409	-0.6699
O	1.8419	4.4235	-0.6533	O	1.2475	4.4381	-0.7254
N	-1.2628	-3.1717	0.8299	N	-1.2628	-3.2503	0.8786
O	-1.4774	-4.4689	0.8855	O	-1.4774	-4.5475	0.9342
O	0.6502	3.2919	1.4034	O	1.1747	3.131	1.5587
O	0.9467	-3.4618	0.6852	O	0.9467	-3.5404	0.7338
H	2.3572	-1.6399	0.5298	H	2.3572	-1.7185	0.5785
H	-1.3378	1.5284	0.6886	H	-1.3378	1.4498	0.7373
H	1.9235	2.5313	-1.3608	H	0.8897	2.6147	-1.5224
H	2.2712	4.7982	-1.4034	H	1.2677	4.8769	-1.5587
H	-2.0428	-2.5279	0.864	H	-2.0428	-2.6065	0.9127
H	-2.3572	-4.7982	0.957	H	-2.3572	-4.8769	1.0057
120°				**150°**			
N	1.844	0.246	0.4716	N	1.844	0.1739	0.2733
C	1.5395	-1.0705	0.5337	C	1.5395	-1.1426	0.3354
C	0.236	-1.5272	0.6387	C	0.236	-1.5993	0.4404
N	-0.8245	-0.6888	0.6863	N	-0.8245	-0.7609	0.488
C	-0.5201	0.6278	0.6242	C	-0.5201	0.5557	0.4259
C	0.7834	1.0844	0.5192	C	0.7834	1.0123	0.3209
C	0.0157	-2.8589	0.6957	C	0.0157	-2.931	0.4974
C	1.0037	2.4161	0.4622	C	1.0037	2.344	0.2639
N	0.4605	3.1569	-0.5529	N	0.0636	3.1702	-0.291
O	0.6751	4.4541	-0.6084	O	0.2782	4.4674	-0.3465
N	-1.2628	-3.3373	0.7997	N	-1.2628	-3.4094	0.6013
O	-1.4774	-4.6345	0.8552	O	-1.4774	-4.7066	0.6569
O	1.6798	2.9531	1.3069	O	2.03	2.8057	0.7026
O	0.9467	-3.6274	0.6549	O	0.9467	-3.6995	0.4565
H	2.3572	-1.8055	0.4995	H	2.3572	-1.8776	0.3012
H	-1.3378	1.3628	0.6583	H	-1.3378	1.2907	0.46
H	-0.1058	2.707	-1.2606	H	-0.7962	2.7834	-0.6586
H	0.3015	4.9639	-1.3069	H	-0.3686	5.0359	-0.7284
H	-2.0428	-2.6935	0.8338	H	-2.0428	-2.7656	0.6354
H	-2.3572	-4.9639	0.9268	H	-2.3572	-5.0359	0.7284
180°				**210°**			

N	1.844	0.1361	-0.177	N	1.844	0.1427	-0.2552
C	1.5395	-1.1804	-0.1149	C	1.5395	-1.1738	-0.1931
C	0.236	-1.6371	-0.0099	C	0.236	-1.6305	-0.0881
N	-0.8245	-0.7987	0.0377	N	-0.8245	-0.7921	-0.0405
C	-0.5201	0.5179	-0.0244	C	-0.5201	0.5245	-0.1026
C	0.7834	0.9745	-0.1294	C	0.7834	0.9811	-0.2076
C	0.0157	-2.9688	0.0471	C	0.0157	-2.9622	-0.0311
C	1.0037	2.3062	-0.1864	C	1.0037	2.3128	-0.2646
N	-0.0515	3.1772	-0.1401	N	0.146	3.176	0.3627
O	0.1631	4.4744	-0.1956	O	0.3606	4.4732	0.3072
N	-1.2628	-3.4472	0.151	N	-1.2628	-3.4406	0.0729
O	-1.4774	-4.7444	0.2066	O	-1.4774	-4.7378	0.1284
O	2.1317	2.7284	-0.2781	O	1.9574	2.7419	-0.8689
O	0.9467	-3.7373	0.0062	O	0.9467	-3.7307	-0.0719
H	2.3572	-1.9154	-0.1491	H	2.3572	-1.9088	-0.2273
H	-1.3378	1.2529	0.0097	H	-1.3378	1.2595	-0.0685
H	-0.9965	2.8235	-0.0634	H	-0.6531	2.8165	0.8689
H	-0.563	5.0737	-0.1639	H	-0.2297	5.0671	0.7387
H	-2.0428	-2.8034	0.1851	H	-2.0428	-2.7968	0.107
H	-2.3572	-5.0737	0.2781	H	-2.3572	-5.0671	0.2
240°				**270°**			
N	1.844	0.1919	-0.4288	N	1.844	0.2705	-0.4806
C	1.5395	-1.1246	-0.3667	C	1.5395	-1.046	-0.4185
C	0.236	-1.5813	-0.2617	C	0.236	-1.5027	-0.3135
N	-0.8245	-0.7429	-0.2141	N	-0.8245	-0.6643	-0.2659
C	-0.5201	0.5737	-0.2762	C	-0.5201	0.6523	-0.328
C	0.7834	1.0303	-0.3812	C	0.7834	1.1089	-0.433
C	0.0157	-2.913	-0.2047	C	0.0157	-2.8344	-0.2565
C	1.0037	2.362	-0.4382	C	1.0037	2.4406	-0.49
N	0.6032	3.1669	0.5943	N	1.1977	3.1524	0.6633
O	0.8178	4.4641	0.5388	O	1.4123	4.4496	0.6078
N	-1.2628	-3.3914	-0.1007	N	-1.2628	-3.3128	-0.1525
O	-1.4774	-4.6886	-0.0452	O	-1.4774	-4.61	-0.097
O	1.5541	2.8425	-1.4001	O	1.0296	3.0033	-1.5585
O	0.9467	-3.6815	-0.2455	O	0.9467	-3.6029	-0.2973
H	2.3572	-1.8596	-0.4009	H	2.3572	-1.781	-0.4527
H	-1.3378	1.3087	-0.2421	H	-1.3378	1.3873	-0.2939
H	0.142	2.7644	1.4001	H	1.1759	2.681	1.5585
H	0.5422	5.0179	1.2492	H	1.5456	4.9393	1.4014
H	-2.0428	-2.7476	-0.0666	H	-2.0428	-2.669	-0.1184
H	-2.3572	-5.0179	0.0264	H	-2.3572	-4.9393	-0.0254
300°				**330°**			
N	1.7666	0.3575	-0.3966	N	1.4316	0.4296	-0.1995
C	1.4621	-0.959	-0.3345	C	1.1271	-0.8869	-0.1374
C	0.1586	-1.4157	-0.2295	C	-0.1764	-1.3436	-0.0324

N	-0.9019	-0.5773	-0.1819	N	-1.2369	-0.5052	0.0152
C	-0.5975	0.7393	-0.244	C	-0.9325	0.8114	-0.0469
C	0.706	1.1959	-0.349	C	0.371	1.268	-0.1519
C	-0.0617	-2.7474	-0.1725	C	-0.3967	-2.6753	0.0246
C	0.9263	2.5276	-0.406	C	0.5913	2.5997	-0.2089
N	1.6927	3.1363	0.5513	N	1.7546	3.123	0.2882
O	1.9073	4.4335	0.4957	O	1.9692	4.4202	0.2327
N	-1.3402	-3.2258	-0.0686	N	-1.6753	-3.1537	0.1286
O	-1.5548	-4.523	-0.013	O	-1.8898	-4.4509	0.1841
O	0.4472	3.1813	-1.3017	O	-0.2381	3.3287	-0.6985
O	0.8693	-3.5159	-0.2134	O	0.5343	-3.4438	-0.0162
H	2.2798	-1.694	-0.3687	H	1.9448	-1.6219	-0.1716
H	-1.4152	1.4743	-0.2099	H	-1.7502	1.5464	-0.0128
H	2.094	2.5887	1.3017	H	2.4493	2.5123	0.6985
H	2.4345	4.8523	1.1545	H	2.7696	4.7802	0.5749
H	-2.1202	-2.582	-0.0345	H	-2.4552	-2.5099	0.1627
H	-2.4345	-4.8523	0.0585	H	-2.7696	-4.7802	0.2557

Table S30 Cartesian coordinates of the PZDH ligand geometry after co-rotation of both hydroxamate groups.

0°				**30°**			
N	1.3343	0.4674	-0.1073	N	1.3343	0.4674	-0.1073
C	1.0298	-0.8491	-0.0452	C	1.0298	-0.8491	-0.0452
C	-0.2737	-1.3058	0.0598	C	-0.2737	-1.3058	0.0598
N	-1.3342	-0.4674	0.1074	N	-1.3342	-0.4674	0.1074
C	-1.0298	0.8492	0.0453	C	-1.0298	0.8492	0.0453
C	0.2737	1.3058	-0.0597	C	0.2737	1.3058	-0.0597
C	-0.494	-2.6375	0.1168	C	-0.494	-2.6375	0.1168
C	0.494	2.6375	-0.1167	C	0.494	2.6375	-0.1167
N	1.7725	3.116	-0.2208	N	1.575	3.1238	-0.8018
O	1.9871	4.4132	-0.2764	O	1.7895	4.421	-0.8574
N	-1.7725	-3.1159	0.2207	N	-1.575	-3.1237	0.8018
O	-1.987	-4.4131	0.2763	O	-1.7895	-4.4209	0.8573
O	-0.437	3.406	-0.076	O	-0.2628	3.3991	0.4366
O	0.4371	-3.406	0.0759	O	0.2628	-3.3991	-0.4368
H	1.8475	-1.5841	-0.0794	H	1.8475	-1.5841	-0.0794
H	-1.8475	1.5842	0.0794	H	-1.8475	1.5842	0.0794
H	2.5525	2.4722	-0.2548	H	2.2091	2.4858	-1.2653
H	2.8668	4.7424	-0.3478	H	2.5334	4.7556	-1.3286
H	-2.5524	-2.4721	0.2548	H	-2.209	-2.4857	1.2653
H	-2.8668	-4.7424	0.3478	H	-2.5334	-4.7556	1.3286
60°				**90°**			
N	1.3343	0.4674	-0.1073	N	1.3343	0.4674	-0.1073

C	1.0298	-0.8491	-0.0452	C	1.0298	-0.8491	-0.0452
C	-0.2737	-1.3058	0.0598	C	-0.2737	-1.3058	0.0598
N	-1.3342	-0.4674	0.1074	N	-1.3342	-0.4674	0.1074
C	-1.0298	0.8492	0.0453	C	-1.0298	0.8492	0.0452
C	0.2737	1.3058	-0.0597	C	0.2737	1.3058	-0.0597
C	-0.494	-2.6375	0.1168	C	-0.494	-2.6375	0.1168
C	0.494	2.6375	-0.1167	C	0.494	2.6375	-0.1167
N	1.1177	3.1821	-1.207	N	0.5232	3.2753	-1.3278
O	1.3322	4.4793	-1.2626	O	0.7377	4.5725	-1.3834
N	-1.1178	-3.182	1.207	N	-0.5234	-3.2752	1.3279
O	-1.3323	-4.4792	1.2625	O	-0.7379	-4.5724	1.3833
O	0.1406	3.3477	0.7942	O	0.665	3.2655	0.9008
O	-0.1407	-3.3477	-0.7943	O	-0.6652	-3.2655	-0.9009
H	1.8475	-1.5841	-0.0794	H	1.8475	-1.5841	-0.0794
H	-1.8475	1.5842	0.0794	H	-1.8475	1.5842	0.0794
H	1.4139	2.5871	-1.9701	H	0.38	2.7492	-2.1803
H	1.7615	4.854	-2.0127	H	0.758	5.0112	-2.2167
H	-1.4139	-2.587	1.9701	H	-0.3801	-2.7491	2.1802
H	-1.7616	-4.854	2.0127	H	-0.7581	-5.0112	2.2167
120°				**150°**			
N	1.3343	0.4674	-0.1074	N	1.3343	0.4674	-0.1074
C	1.0298	-0.8491	-0.0453	C	1.0298	-0.8491	-0.0453
C	-0.2737	-1.3058	0.0597	C	-0.2737	-1.3058	0.0597
N	-1.3342	-0.4674	0.1073	N	-1.3342	-0.4674	0.1073
C	-1.0298	0.8492	0.0452	C	-1.0298	0.8492	0.0452
C	0.2737	1.3058	-0.0598	C	0.2737	1.3058	-0.0598
C	-0.494	-2.6375	0.1167	C	-0.494	-2.6375	0.1167
C	0.494	2.6375	-0.1168	C	0.494	2.6375	-0.1168
N	-0.0492	3.3784	-1.1319	N	-0.4461	3.4637	-0.6716
O	0.1653	4.6756	-1.1874	O	-0.2316	4.7609	-0.7271
N	0.0491	-3.3782	1.1319	N	0.4461	-3.4636	0.6717
O	-0.1655	-4.6754	1.1873	O	0.2314	-4.7608	0.7271
O	1.1701	3.1746	0.7279	O	1.5203	3.0992	0.3219
O	-1.1703	-3.1745	-0.728	O	-1.5205	-3.0992	-0.3219
H	1.8475	-1.5841	-0.0795	H	1.8475	-1.5841	-0.0795
H	-1.8475	1.5842	0.0793	H	-1.8475	1.5842	0.0793
H	-0.6155	2.9284	-1.8396	H	-1.3059	3.0769	-1.0393
H	-0.2083	5.1853	-1.8859	H	-0.8784	5.3294	-1.1091
H	0.6154	-2.9283	1.8395	H	1.3058	-3.0768	1.0392
H	0.2082	-5.1853	1.8859	H	0.8783	-5.3294	1.1091
180°				**210°**			
N	1.3343	0.4674	-0.1074	N	1.3343	0.4674	-0.1074
C	1.0298	-0.8491	-0.0453	C	1.0298	-0.8491	-0.0453
C	-0.2737	-1.3058	0.0597	C	-0.2737	-1.3058	0.0597
N	-1.3342	-0.4674	0.1073	N	-1.3342	-0.4674	0.1073

C	-1.0298	0.8492	0.0452	C	-1.0298	0.8492	0.0452
C	0.2737	1.3058	-0.0598	C	0.2737	1.3058	-0.0598
C	-0.494	-2.6375	0.1167	C	-0.494	-2.6375	0.1167
C	0.494	2.6375	-0.1168	C	0.494	2.6375	-0.1168
N	-0.5613	3.5085	-0.0705	N	-0.3638	3.5007	0.5106
O	-0.3467	4.8057	-0.126	O	-0.1492	4.7979	0.4551
N	0.5613	-3.5084	0.0705	N	0.3638	-3.5006	-0.5105
O	0.3466	-4.8056	0.126	O	0.1491	-4.7978	-0.455
O	1.622	3.0597	-0.2085	O	1.4478	3.0666	-0.7211
O	-1.6221	-3.0597	0.2085	O	-1.4478	-3.0666	0.7212
H	1.8475	-1.5841	-0.0795	H	1.8475	-1.5841	-0.0795
H	-1.8475	1.5842	0.0793	H	-1.8475	1.5842	0.0793
H	-1.5063	3.1548	0.0062	H	-1.1629	3.1412	1.0168
H	-1.0728	5.405	-0.0943	H	-0.7394	5.3918	0.8866
H	1.5062	-3.1547	-0.0063	H	1.1628	-3.1411	-1.0168
H	1.0728	-5.405	0.0942	H	0.7394	-5.3918	-0.8866
240°				**270°**			
N	1.3343	0.4674	-0.1074	N	1.3343	0.4674	-0.1074
C	1.0298	-0.8491	-0.0453	C	1.0298	-0.8491	-0.0453
C	-0.2737	-1.3058	0.0597	C	-0.2737	-1.3058	0.0597
N	-1.3342	-0.4674	0.1073	N	-1.3342	-0.4674	0.1073
C	-1.0298	0.8492	0.0452	C	-1.0298	0.8492	0.0452
C	0.2737	1.3058	-0.0598	C	0.2737	1.3058	-0.0598
C	-0.494	-2.6375	0.1167	C	-0.494	-2.6375	0.1167
C	0.494	2.6375	-0.1168	C	0.494	2.6375	-0.1168
N	0.0935	3.4424	0.9158	N	0.688	3.3492	1.0366
O	0.3081	4.7396	0.8603	O	0.9026	4.6464	0.981
N	-0.0934	-3.4423	-0.9158	N	-0.6879	-3.3491	-1.0367
O	-0.3081	-4.7395	-0.8602	O	-0.9025	-4.6463	-0.981
O	1.0444	3.118	-1.0787	O	0.5199	3.2002	-1.1853
O	-1.0444	-3.118	1.0787	O	-0.5198	-3.2002	1.1853
H	1.8475	-1.5841	-0.0795	H	1.8475	-1.5841	-0.0795
H	-1.8475	1.5842	0.0793	H	-1.8475	1.5842	0.0793
H	-0.3677	3.0399	1.7215	H	0.6662	2.8778	1.9317
H	0.0324	5.2934	1.5706	H	1.036	5.1361	1.7746
H	0.3677	-3.0398	-1.7215	H	-0.6662	-2.8777	-1.9317
H	-0.0324	-5.2934	-1.5707	H	-1.036	-5.1361	-1.7747
300°				**330°**			
N	1.3343	0.4674	-0.1074	N	1.3343	0.4674	-0.1074
C	1.0298	-0.8491	-0.0453	C	1.0298	-0.8491	-0.0453
C	-0.2737	-1.3058	0.0597	C	-0.2737	-1.3058	0.0597
N	-1.3342	-0.4674	0.1073	N	-1.3342	-0.4674	0.1073
C	-1.0298	0.8492	0.0452	C	-1.0298	0.8492	0.0452
C	0.2737	1.3058	-0.0598	C	0.2737	1.3058	-0.0598
C	-0.494	-2.6375	0.1167	C	-0.494	-2.6375	0.1167

C	0.494	2.6375	-0.1168	C	0.494	2.6375	-0.1168
N	1.2604	3.2461	0.8406	N	1.6574	3.1608	0.3804
O	1.475	4.5433	0.785	O	1.872	4.458	0.3248
N	-1.2603	-3.2461	-0.8407	N	-1.6573	-3.1607	-0.3805
O	-1.4749	-4.5433	-0.7851	O	-1.8718	-4.4579	-0.3249
O	0.0149	3.2912	-1.0125	O	-0.3354	3.3665	-0.6064
O	-0.0147	-3.2912	1.0124	O	0.3355	-3.3665	0.6063
H	1.8475	-1.5841	-0.0795	H	1.8475	-1.5841	-0.0795
H	-1.8475	1.5842	0.0793	H	-1.8475	1.5842	0.0793
H	1.6617	2.6986	1.591	H	2.3522	2.5501	0.7907
H	2.0023	4.9621	1.4439	H	2.6724	4.818	0.667
H	-1.6616	-2.6985	-1.591	H	-2.3521	-2.55	-0.7907
H	-2.0023	-4.9621	-1.444	H	-2.6724	-4.818	-0.6671

Table S31 Cartesian coordinates of the PZDH ligand geometry after counter-rotation of both hydroxamate groups.

0°				**30°**			
N	1.3343	0.4674	-0.1073	N	0.7512	0.4419	1.6634
C	1.0298	-0.8491	-0.0452	C	1.357	-0.7009	1.2673
C	-0.2737	-1.3058	0.0598	C	0.752	-1.6027	0.4073
N	-1.3342	-0.4674	0.1074	N	-0.4872	-1.404	-0.0972
C	-1.0298	0.8492	0.0453	C	-1.0931	-0.2612	0.2988
C	0.2737	1.3058	-0.0597	C	-0.4881	0.6405	1.1587
C	-0.494	-2.6375	0.1168	C	1.4244	-2.7218	0.0598
C	0.494	2.6375	-0.1167	C	-1.1604	1.7596	1.5063
N	1.7725	3.116	-0.2208	N	-0.474	2.9069	1.8007
O	1.9871	4.4132	-0.2764	O	-1.1289	3.997	2.1393
N	-1.7725	-3.1159	0.2207	N	1.2071	-3.2991	-1.1624
O	-1.987	-4.4131	0.2763	O	1.862	-4.3892	-1.5009
O	-0.437	3.406	-0.076	O	-2.3673	1.7479	1.5573
O	0.4371	-3.406	0.0759	O	2.2173	-3.213	0.8274
H	1.8475	-1.5841	-0.0794	H	2.3673	-0.9223	1.6419
H	-1.8475	1.5842	0.0794	H	-2.1034	-0.0399	-0.0758
H	2.5525	2.4722	-0.2548	H	0.5371	2.9167	1.758
H	2.8668	4.7424	-0.3478	H	-0.6566	4.7865	2.3419
H	-2.5524	-2.4721	0.2548	H	0.5428	-2.8876	-1.8055
H	-2.8668	-4.7424	0.3478	H	1.7125	-4.7865	-2.3419
60°				**90°**			
N	0.579	0.0897	1.8762	N	0.0798	-0.0382	1.4943
C	1.1847	-1.0531	1.4801	C	0.6856	-1.181	1.0982
C	0.5797	-1.9549	0.6202	C	0.0806	-2.0828	0.2382
N	-0.6595	-1.7562	0.1156	N	-1.1587	-1.8841	-0.2663
C	-1.2654	-0.6134	0.5116	C	-1.7645	-0.7413	0.1297

C	-0.6604	0.2883	1.3716	C	-1.1595	0.1604	0.9897
C	1.2521	-3.074	0.2726	C	0.7529	-3.2018	-0.1093
C	-1.3327	1.4074	1.7191	C	-1.8318	1.2795	1.3372
N	-0.8095	2.6385	1.4279	N	-1.7033	2.4165	0.5856
O	-1.4644	3.7286	1.7665	O	-2.3583	3.5066	0.9241
N	1.5415	-3.3178	-1.043	N	1.5627	-3.1989	-1.2131
O	2.1964	-4.4079	-1.3816	O	2.2176	-4.289	-1.5517
O	-2.3955	1.3217	2.2869	O	-2.5464	1.2769	2.3112
O	1.5979	-3.8594	1.1228	O	0.6396	-4.2051	0.5539
H	2.195	-1.2744	1.8548	H	1.6958	-1.4023	1.4728
H	-2.2757	-0.392	0.137	H	-2.7748	-0.5199	-0.2449
H	0.0809	2.7103	0.9523	H	-1.1047	2.4187	-0.2304
H	-1.1044	4.5758	1.5661	H	-2.2698	4.289	0.407
H	1.2517	-2.6598	-1.7552	H	1.6577	-2.3584	-1.7688
H	2.3955	-4.5758	-2.2869	H	2.7748	-4.2869	-2.3112
120°				**150°**			
N	-0.0666	0.1698	1.0122	N	0.2233	0.4464	0.5592
C	0.5392	-0.973	0.6161	C	0.829	-0.6964	0.1631
C	-0.0658	-1.8748	-0.2438	C	0.2241	-1.5981	-0.6969
N	-1.3051	-1.6761	-0.7484	N	-1.0152	-1.3994	-1.2015
C	-1.9109	-0.5333	-0.3524	C	-1.6211	-0.2566	-0.8054
C	-1.3059	0.3684	0.5076	C	-1.016	0.6451	0.0545
C	0.6065	-2.9939	-0.5914	C	0.8964	-2.7172	-1.0444
C	-1.9782	1.4875	0.8551	C	-1.6884	1.7642	0.4021
N	-2.3701	2.3776	-0.1083	N	-2.5869	2.3208	-0.4679
O	-3.0251	3.4677	0.2302	O	-3.2419	3.411	-0.1293
N	1.811	-2.8968	-1.2348	N	2.2641	-2.7039	-1.1022
O	2.4659	-3.9869	-1.5733	O	2.919	-3.794	-1.4408
O	-2.2336	1.7027	2.0161	O	-1.4966	2.2736	1.4805
O	0.1449	-4.0802	-0.3344	O	0.2907	-3.7296	-1.3042
H	1.5494	-1.1944	0.9907	H	1.8393	-0.9177	0.5377
H	-2.9212	-0.312	-0.727	H	-2.6314	-0.0353	-1.18
H	-2.1562	2.1973	-1.0809	H	-2.7476	1.8941	-1.3713
H	-3.2947	4.0802	-0.4327	H	-3.8602	3.794	-0.7279
H	2.1978	-1.9867	-1.4501	H	2.7715	-1.8558	-0.8846
H	3.2947	-3.92	-2.0161	H	3.8602	-3.7848	-1.4805
180°				**210°**			
N	0.6193	0.9229	0.8804	N	1.0152	1.3994	1.2015
C	1.225	-0.2198	0.4843	C	1.621	0.2567	0.8054
C	0.62	-1.1216	-0.3757	C	1.016	-0.6451	-0.0545
N	-0.6192	-0.9229	-0.8803	N	-0.2233	-0.4464	-0.5591
C	-1.2251	0.2199	-0.4842	C	-0.8291	0.6964	-0.1631
C	-0.6201	1.1216	0.3757	C	-0.2241	1.5981	0.6969
C	1.2924	-2.2407	-0.7233	C	1.6883	-1.7642	-0.4021
C	-1.2924	2.2407	0.7233	C	-0.8964	2.7172	1.0444

N	-2.5481	2.4667	0.2271	N	-2.2641	2.7039	1.1022
O	-3.2031	3.5568	0.5657	O	-2.9191	3.794	1.4408
N	2.5481	-2.4667	-0.2271	N	2.5869	-2.3209	0.4679
O	3.2031	-3.5568	-0.5657	O	3.2419	-3.411	0.1293
O	-0.7855	3.0419	1.4718	O	-0.2907	3.7296	1.3042
O	0.7855	-3.0419	-1.4718	O	1.4966	-2.2736	-1.4805
H	2.2353	-0.4412	0.8589	H	2.6313	0.0353	1.18
H	-2.2354	0.4412	-0.8589	H	-1.8394	0.9177	-0.5377
H	-2.9728	1.7955	-0.4	H	-2.7716	1.8558	0.8846
H	-4.0671	3.7123	0.2243	H	-3.8602	3.7849	1.4805
H	2.9728	-1.7955	0.4	H	2.7476	-1.8941	1.3713
H	4.0671	-3.7123	-0.2243	H	3.8602	-3.794	0.7279
240°				**270°**			
N	1.3051	1.6761	0.7485	N	1.1587	1.8841	0.2664
C	1.9108	0.5334	0.3524	C	1.7645	0.7413	-0.1297
C	1.3059	-0.3684	-0.5076	C	1.1595	-0.1605	-0.9897
N	0.0666	-0.1697	-1.0122	N	-0.0797	0.0382	-1.4942
C	-0.5393	0.9731	-0.6161	C	-0.6856	1.181	-1.0982
C	0.0658	1.8748	0.2438	C	-0.0806	2.0827	-0.2383
C	1.9782	-1.4875	-0.8551	C	1.8319	-1.2796	-1.3372
C	-0.6066	2.9939	0.5914	C	-0.7529	3.2018	0.1093
N	-1.811	2.8968	1.2348	N	-1.5627	3.1989	1.2131
O	-2.4659	3.9869	1.5733	O	-2.2176	4.289	1.5517
N	2.3701	-2.3776	0.1083	N	1.7034	-2.4165	-0.5856
O	3.0251	-3.4677	-0.2302	O	2.3583	-3.5066	-0.9242
O	-0.1449	4.0802	0.3344	O	-0.6395	4.2051	-0.5539
O	2.2335	-1.7027	-2.0161	O	2.5464	-1.2769	-2.3112
H	2.9211	0.312	0.727	H	2.7748	0.52	0.2449
H	-1.5496	1.1944	-0.9907	H	-1.6959	1.4024	-1.4728
H	-2.1978	1.9867	1.4501	H	-1.6577	2.3584	1.7688
H	-3.2947	3.9201	2.0161	H	-2.7748	4.2869	2.3112
H	2.1562	-2.1973	1.0809	H	1.1048	-2.4187	0.2304
H	3.2947	-4.0802	0.4327	H	2.2699	-4.289	-0.407
300°				**330°**			
N	0.6595	1.7562	-0.1155	N	0.4873	1.404	0.0973
C	1.2653	0.6134	-0.5116	C	1.0931	0.2613	-0.2988
C	0.6603	-0.2883	-1.3716	C	0.4881	-0.6405	-1.1587
N	-0.5789	-0.0897	-1.8762	N	-0.7512	-0.4418	-1.6633
C	-1.1848	1.0532	-1.4801	C	-1.357	0.701	-1.2673
C	-0.5798	1.9549	-0.6202	C	-0.752	1.6027	-0.4073
C	1.3327	-1.4074	-1.7192	C	1.1604	-1.7596	-1.5063
C	-1.2521	3.0739	-0.2726	C	-1.4243	2.7218	-0.0598
N	-1.5415	3.3178	1.043	N	-1.207	3.2991	1.1624
O	-2.1964	4.4079	1.3816	O	-1.8619	4.3892	1.5009
N	0.8095	-2.6385	-1.4279	N	0.474	-2.9069	-1.8007

O	1.4644	-3.7286	-1.7665	O	1.129	-3.997	-2.1393
O	-1.5979	3.8594	-1.1228	O	-2.2172	3.213	-0.8274
O	2.3955	-1.3217	-2.2869	O	2.3673	-1.7479	-1.5573
H	2.2756	0.3921	-0.137	H	2.1034	0.0399	0.0758
H	-2.1951	1.2745	-1.8547	H	-2.3673	0.9223	-1.6419
H	-1.2518	2.6598	1.7552	H	-0.5428	2.8876	1.8055
H	-2.3955	4.5758	2.2869	H	-1.7124	4.7865	2.3419
H	-0.0809	-2.7103	-0.9523	H	-0.537	-2.9167	-1.758
H	1.1044	-4.5758	-1.5661	H	0.6566	-4.7865	-2.3419

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