Electronic supplementary information (ESI)

Pseudotetrahedral Zn(II)-(*R* or *S*)-dihalogen-salicylaldiminato complexes with Λ- or Δ-chirality induction at-metal

Hadi Amiri Rudbari,[a,*] Arezoo Saadati,[a] Mahnaz Aryaeifar,[a] Olivier Blacque,[b] Isabel Correia,[c] Mohammad Khairul Islam,[d] Dennis Woschko,[e] Christoph Janiak,[e,*] and Mohammed Enamullah[d,*]

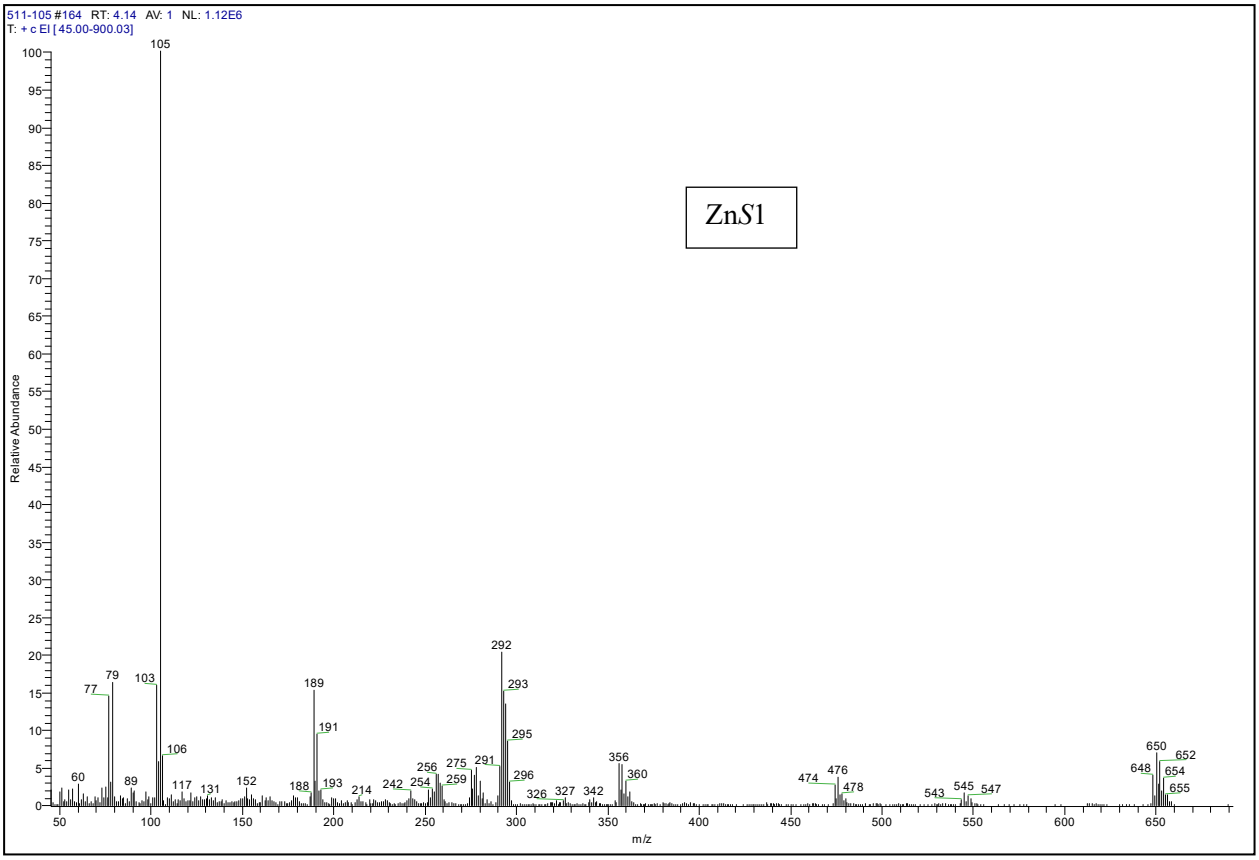
[a] Department of Chemistry, University of Isfahan, Isfahan 81746-73441, Iran.

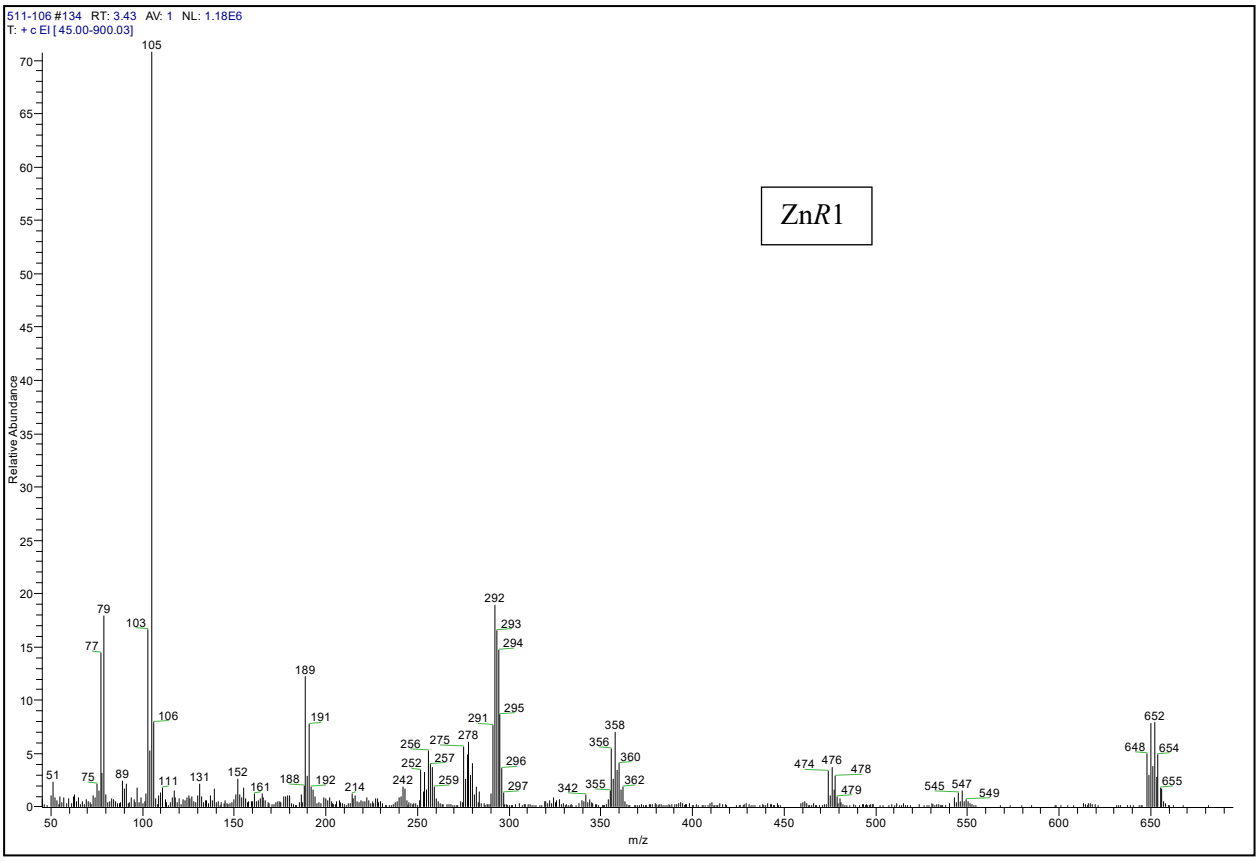
[b] Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057, Zurich, Switzerland.

[c] Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av Rovisco Pais, 1049-001 Lisboa, Portugal.

[d] Department of Chemistry, Jahangirnagar University, Dhaka1342, Bangladesh.

[e] Institut für Anorganische Chemie und Strukturchemie, Universität Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf, Germany.

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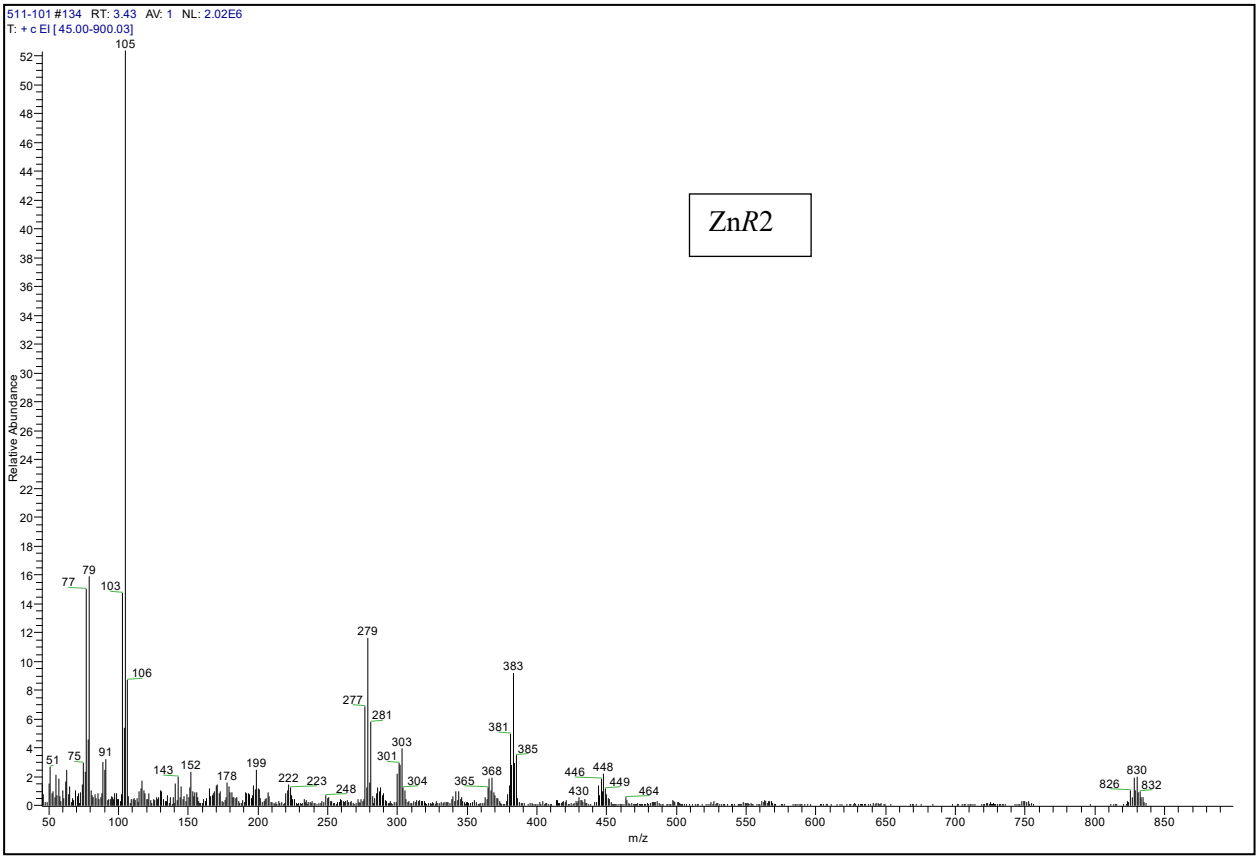
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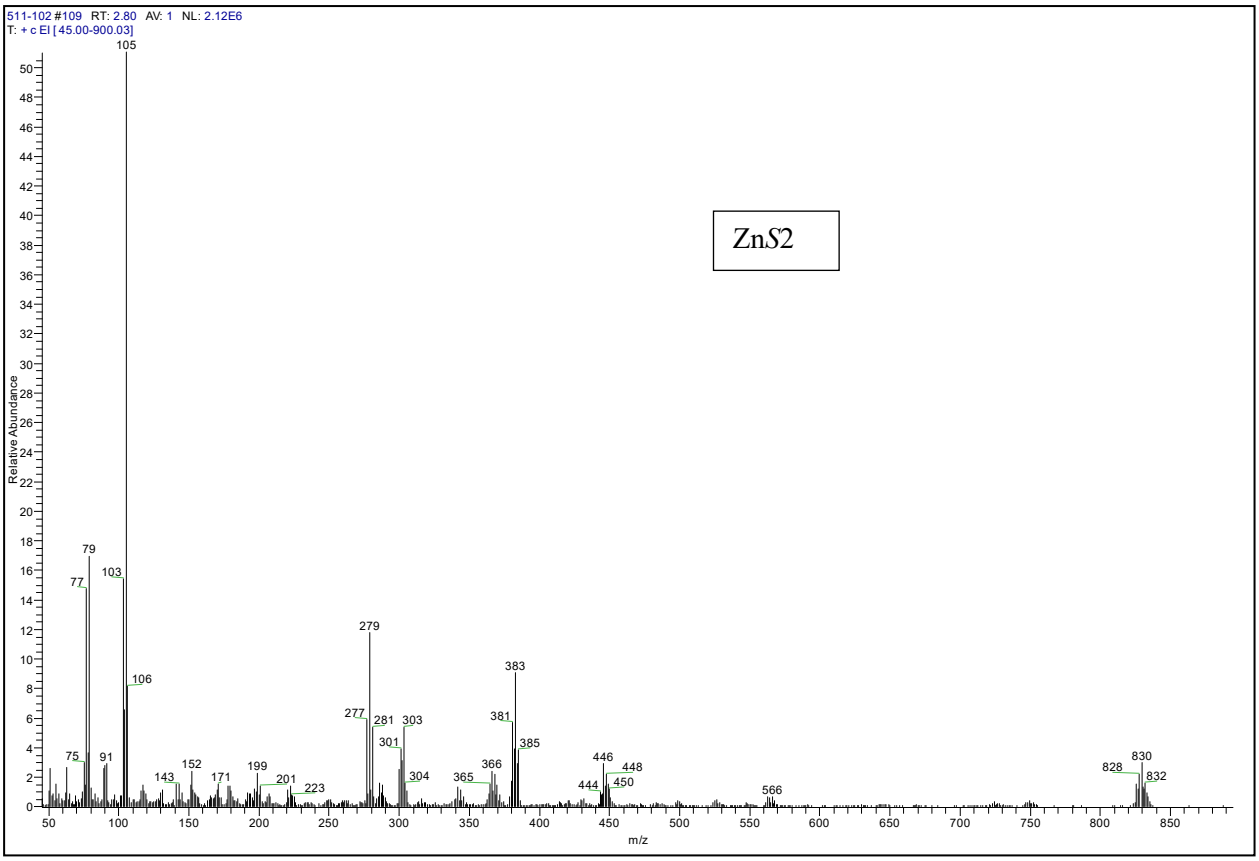
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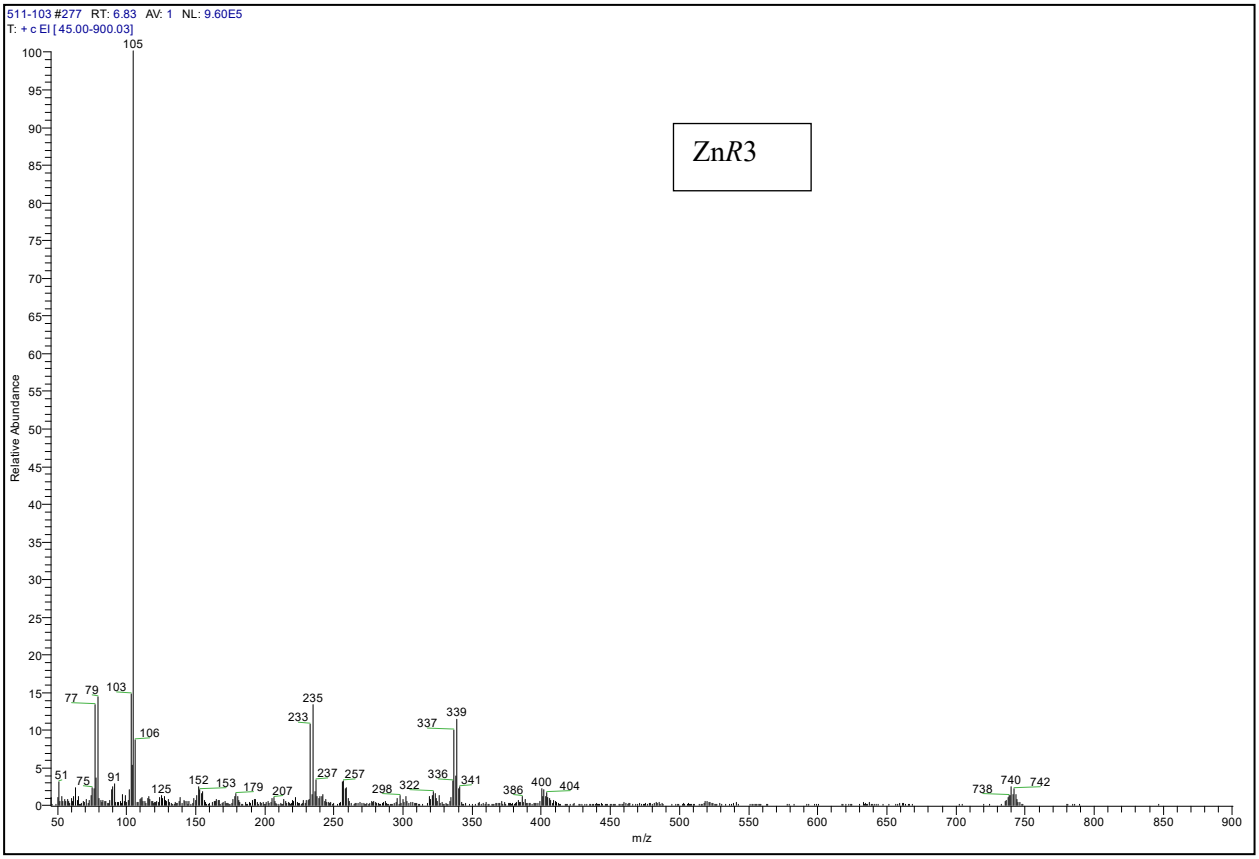
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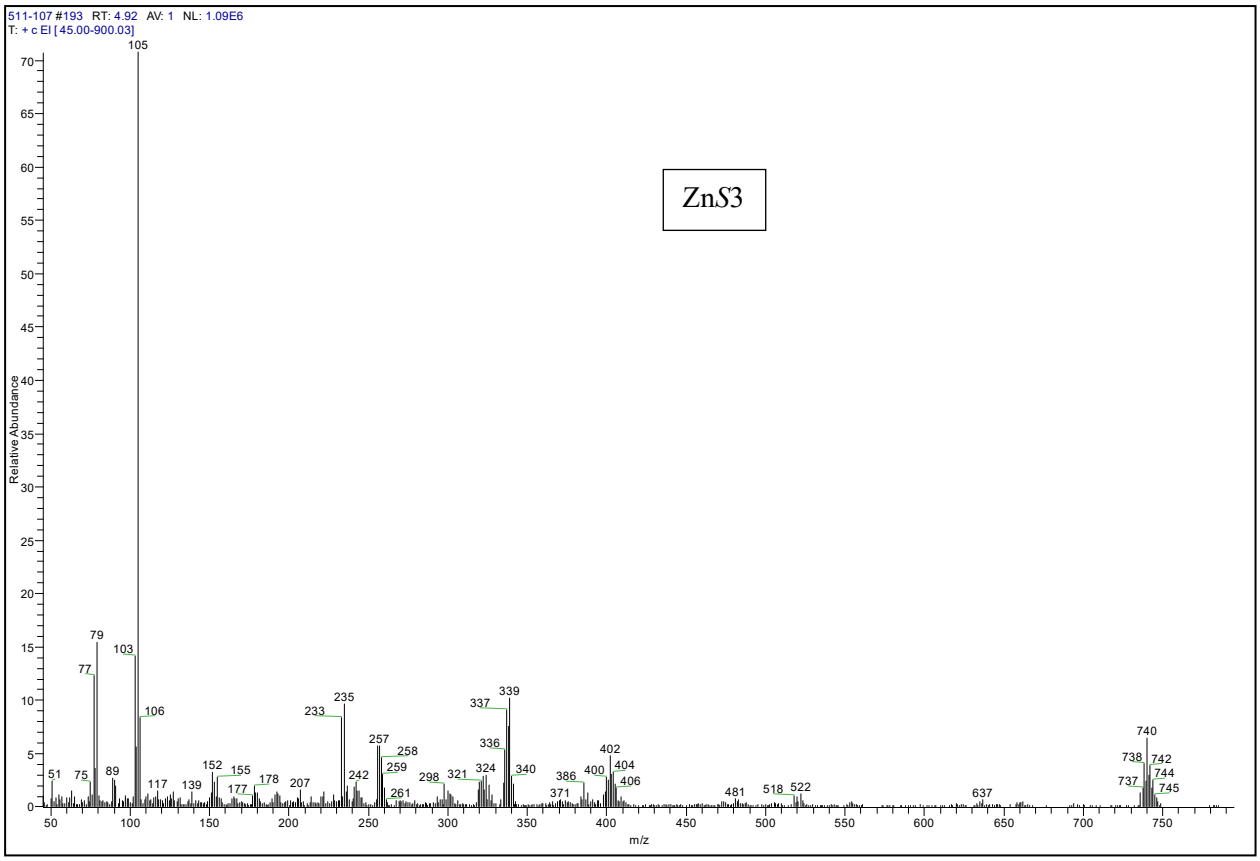
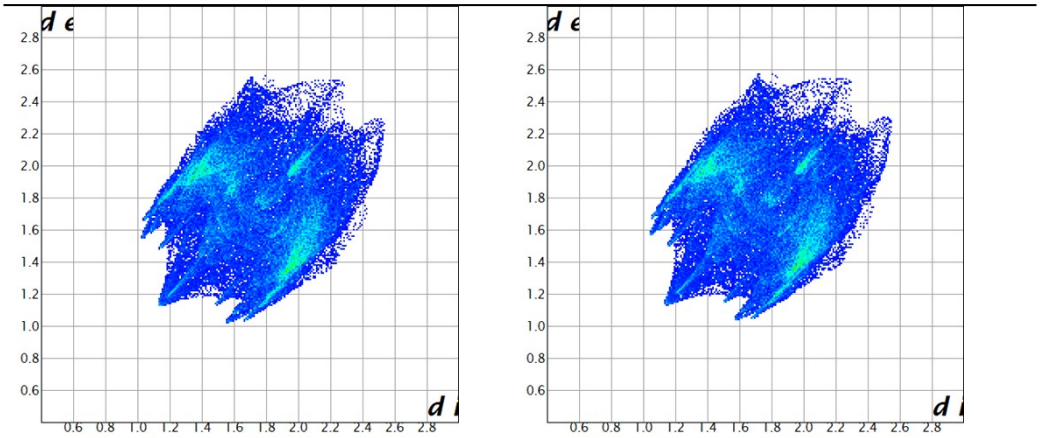
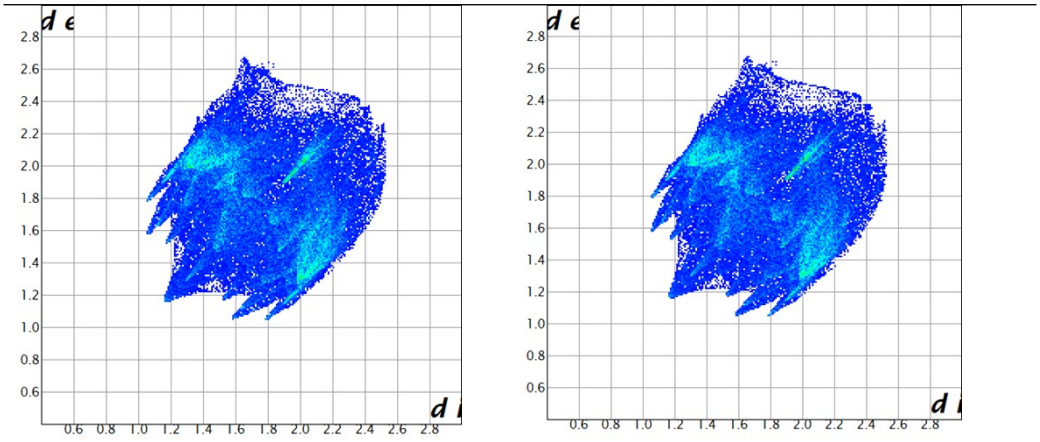
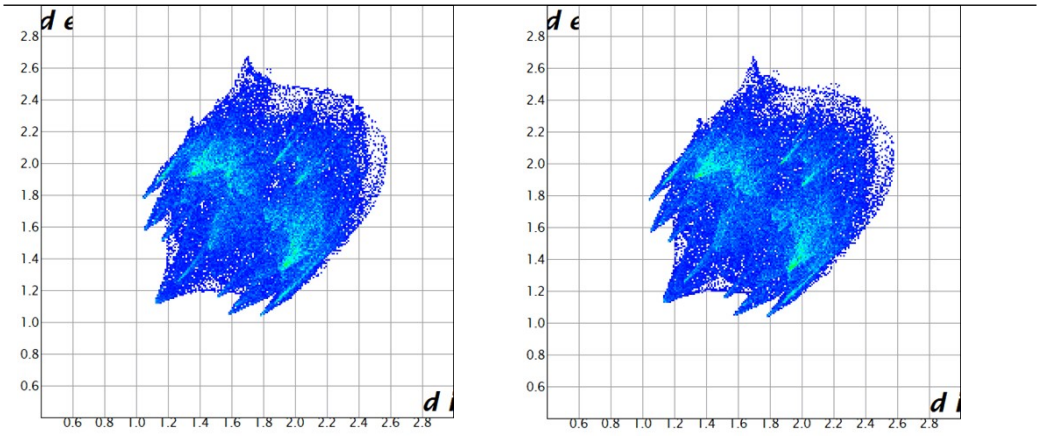


Fig. S1 EI-mass spectra for Zn*R*1-3 and Zn*S*1-3 complexes.



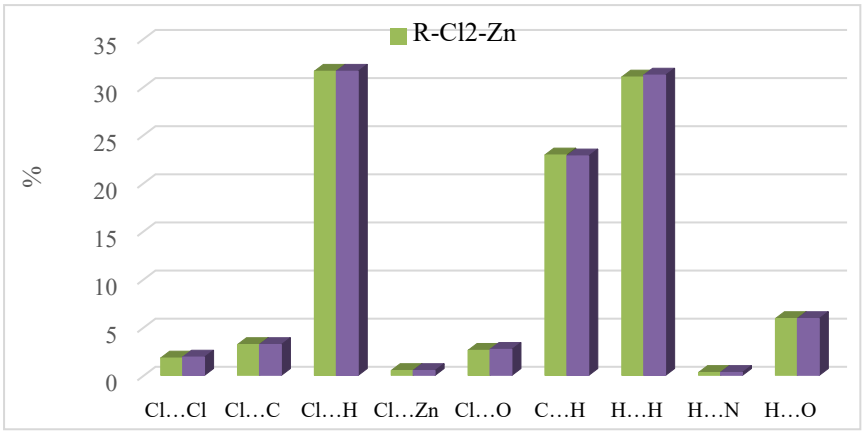


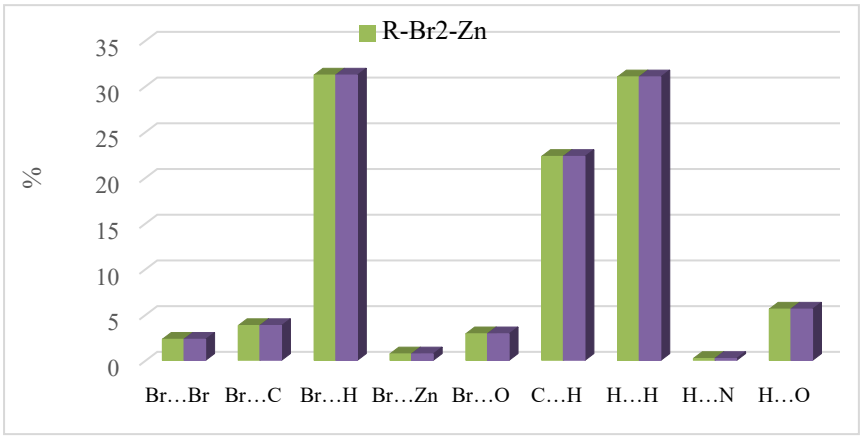
Λ-Zn*R*2 Δ-Zn*S*2



Λ-Zn*R*3 Δ-Zn*S*3

Fig. S2 Two-dimensional fingerprint plots for the Zn(II)-complexes.





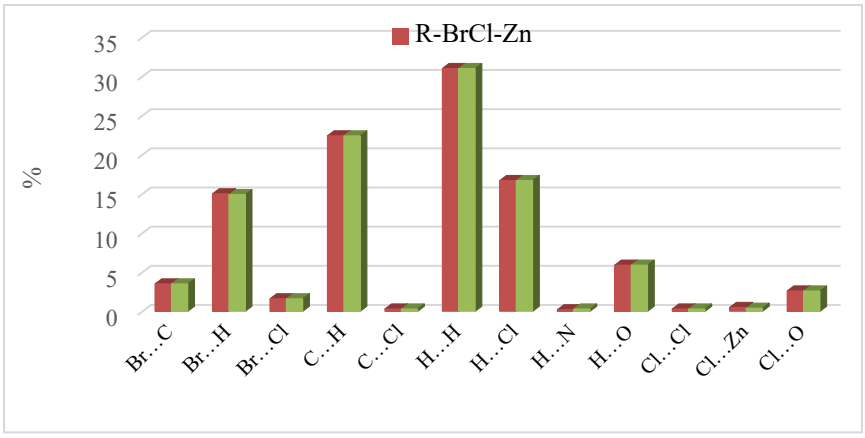


Fig. S3 Relative contributions to the Hirshfeld surfaces area for different intermolecular contacts in Zn(II)-complexes.

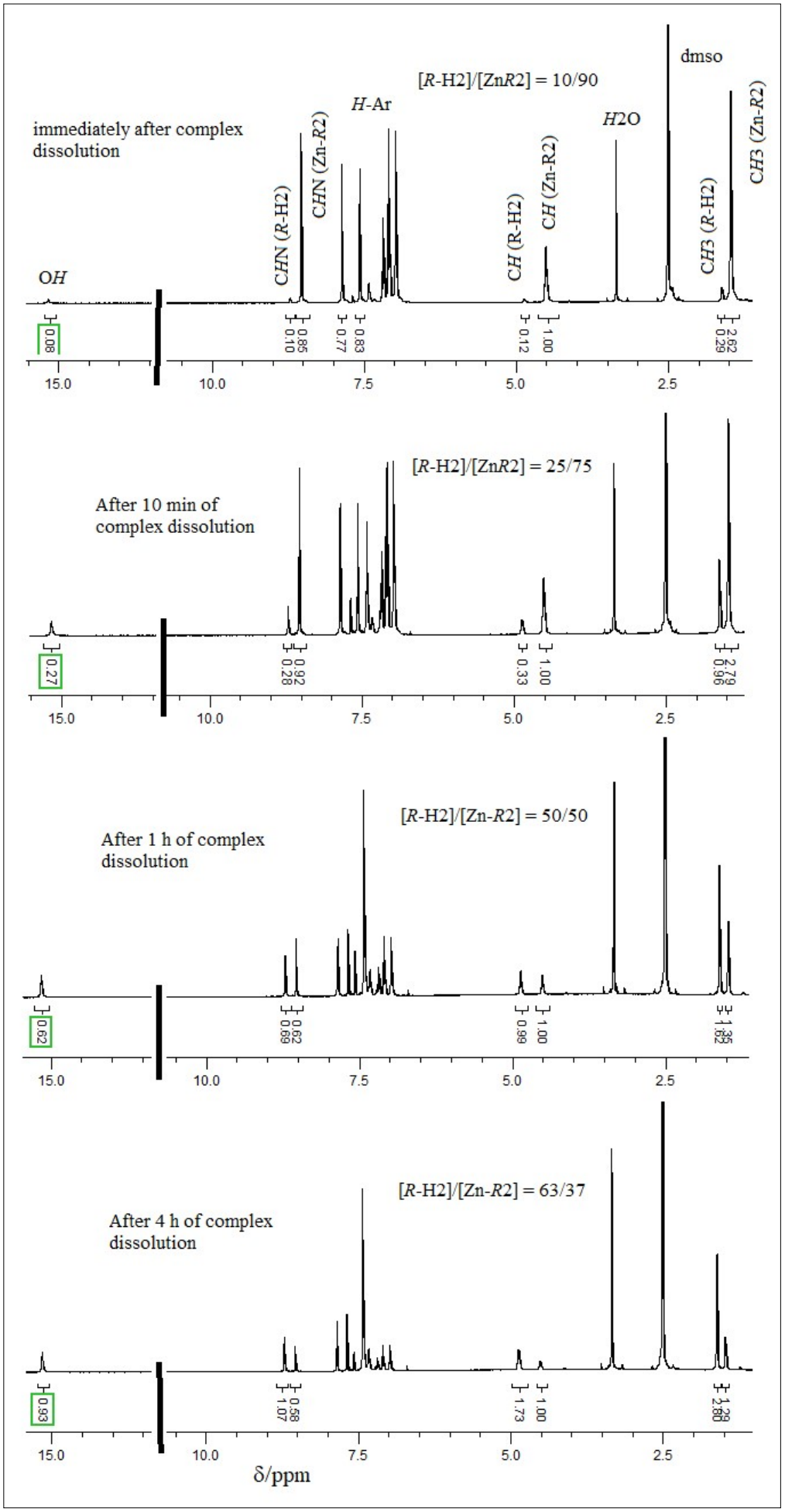
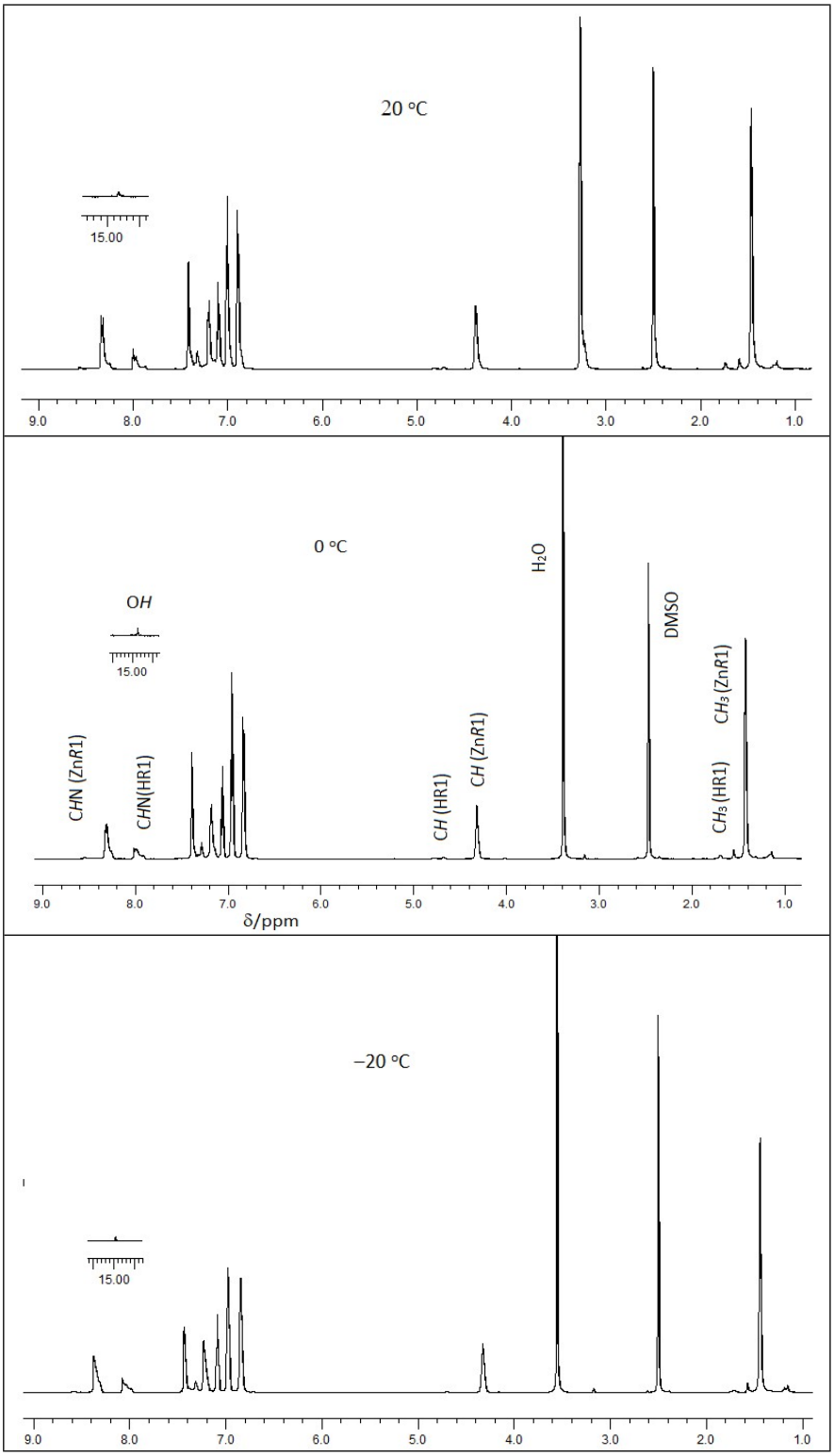

immediately after complex dissolution
[R-H2]/[ZnR2] = 10/90
OH
CHN (R-H2)
CHN (Zn-R2)
H-Ar
CH (R-H2)
CH (Zn-R2)
H2O
dmso
CH3 (R-H2)
CH3 (Zn-R2)
0.08
0.86
0.10
0.77
0.83
0.12
1.00
2.62
0.29
After 10 min of complex dissolution
[R-H2]/[ZnR2] = 25/75
0.27
0.92
0.28
0.33
1.00
2.79
0.96
After 1 h of complex dissolution
[R-H2]/[Zn-R2] = 50/50
0.62
0.62
0.69
0.99
1.00
1.82
After 4 h of complex dissolution
[R-H2]/[Zn-R2] = 63/37
0.93
0.58
1.07
1.73
1.00
2.80
15.0
10.0
7.5
5.0
2.5
δ/ppm

Fig. S4 ^{1}H NMR (400 MHz) spectra for Zn*R*2 with small amounts of extra free Schiff base (*R*-H2) in dmso-d_6 at 25 °C at different time intervals of complex dissolution (single peak corresponds to Λ-Zn*R*2 diastereomer).



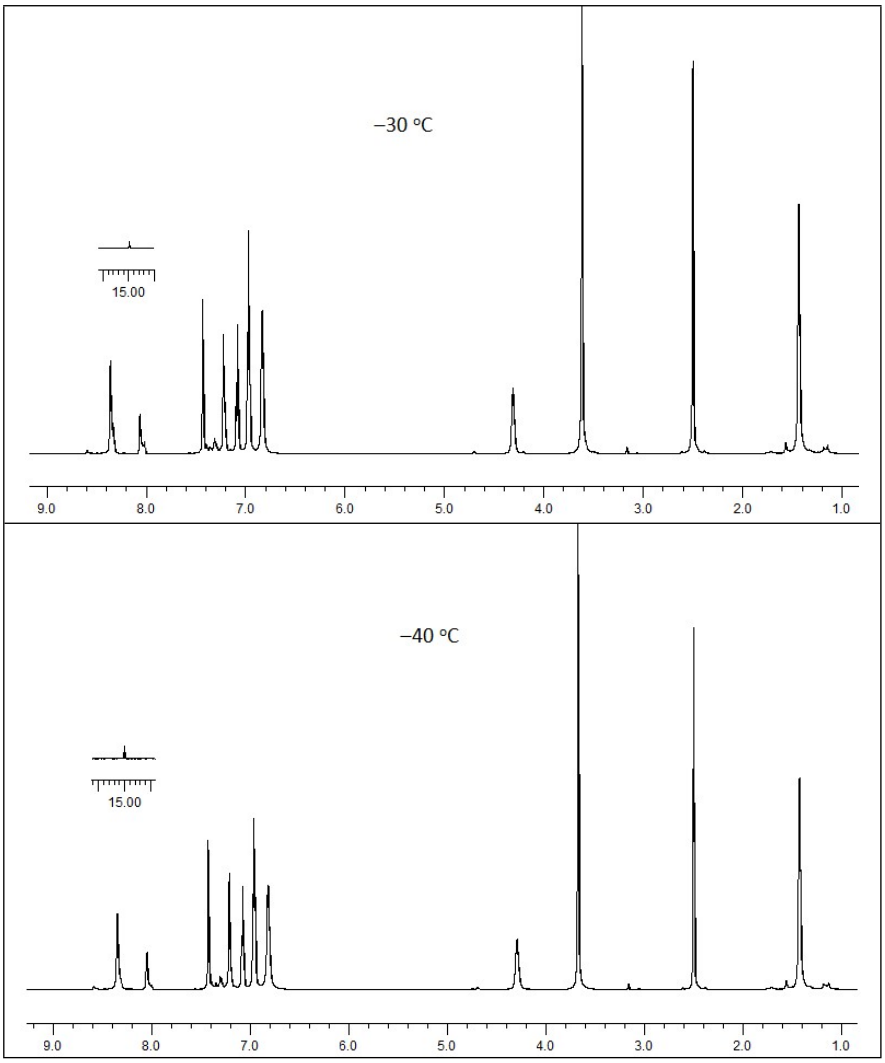


Fig. S5 ^{1}H NMR (400 MHz) spectra for Zn*R*1 at variable temperature (20, 0, –20, –30 and –40 °C) in dmso-d_6/$CDCl_3$ (50%, v/v) (single peak corresponds to Λ-Zn*R*1 diastereomer). Very weak peaks correspond to the Schiff base (<3.0 %), resulting from hydrolysis of the complex with time.

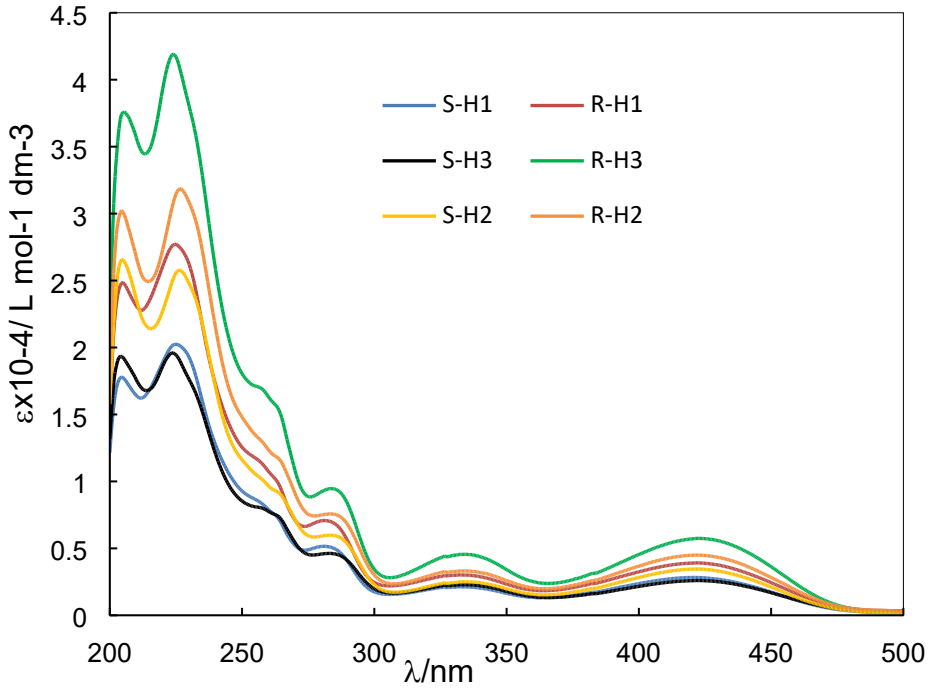


Fig. S6 UV-Vis. spectra for the enantiopure Schiff bases *R*-H1 (3.24×10^{-2} mM), *S*-H1 (3.24×10^{-2} mM), *R*-H2 (2.45×10^{-2} mM), *S*-H2 (3.09×10^{-2} mM), *R*-H3 (2.79×10^{-2} mM) and *S*-H3 (3.10×10^{-2} mM) in methanol at 25 °C.

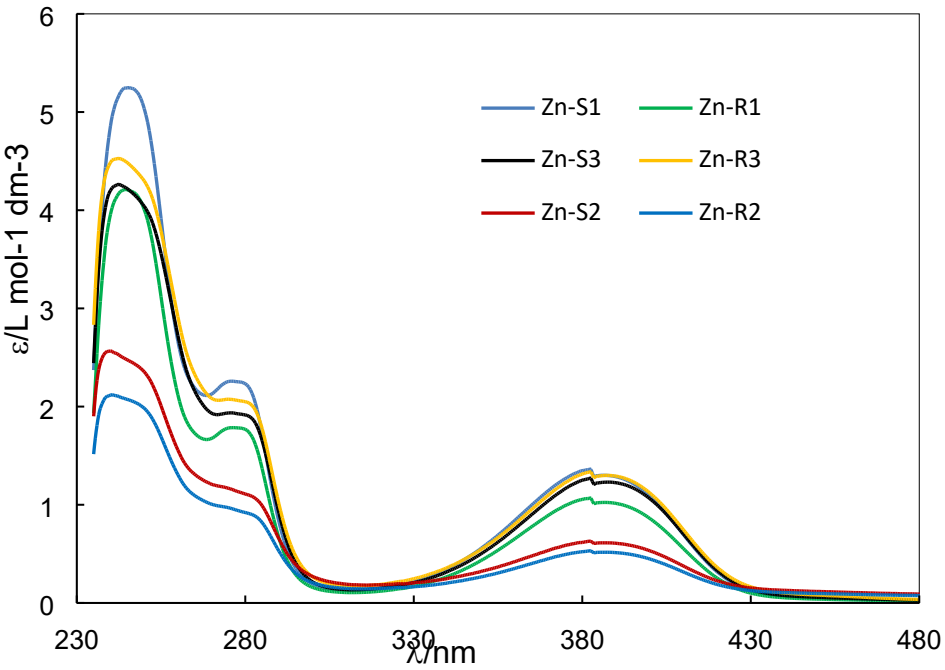


Fig. S7 UV-Vis. spectra for the enantiopure Zn*R*1 (3.89×10^{-2} mM), Zn*S*1 (3.22×10^{-2} mM), Zn*R*2 (2.60×10^{-2} mM), Zn*S*2 (1.58×10^{-2} mM), Zn*R*3 (2.16×10^{-2} mM) and Zn*S*3 (2.97×10^{-2} mM) in methanol/chloroform (50%, v/v) at 25 °C.

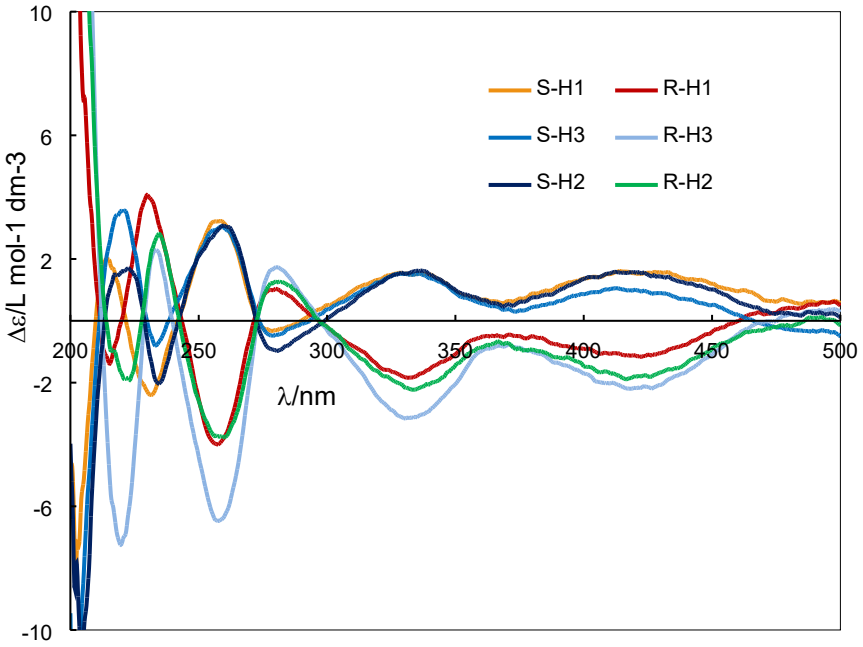
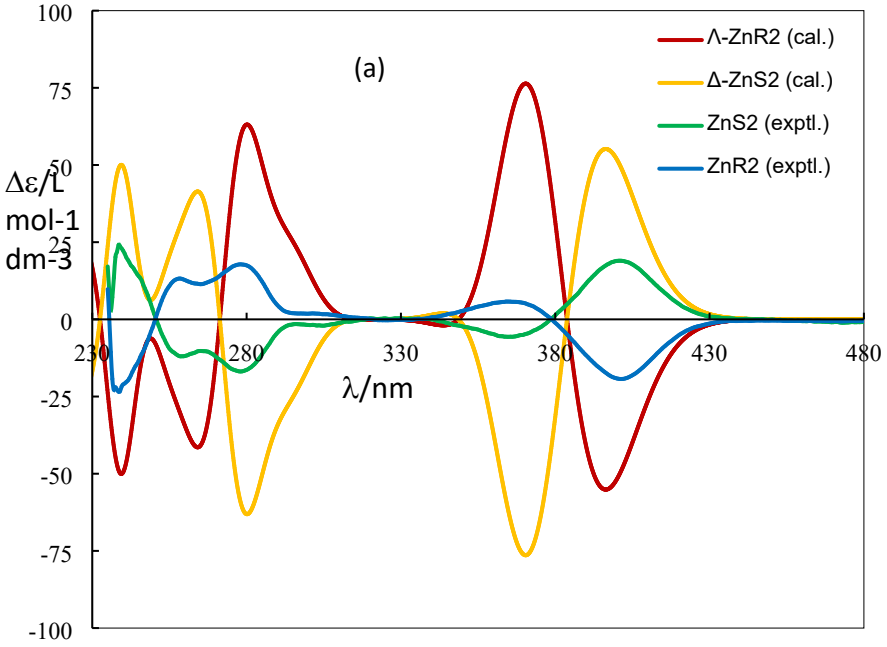


Fig. S8 Electronic circular dichroism (ECD) spectra for enantiomeric pairs of the Schiff bases *R*-H1/*S*-H1, *R*-H2/*S*-H2 and *R*-H3/*S*-H3 (*ca.* 3.00x10^{-2} mM) in methanol at 25 ^{o}C.



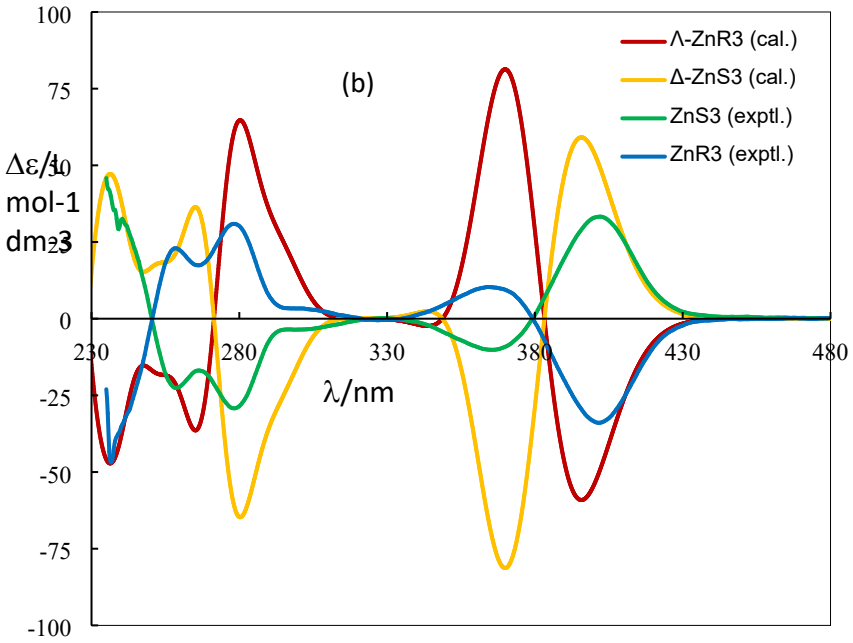
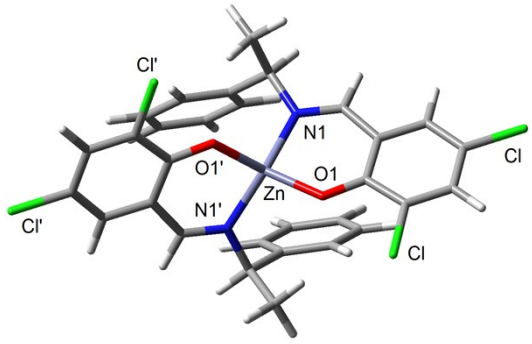
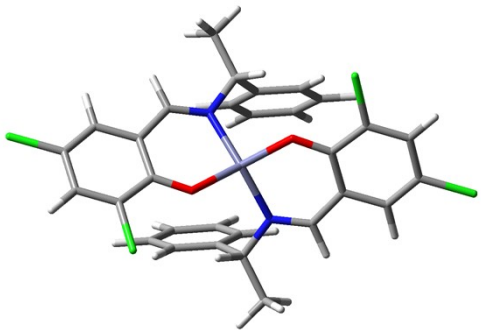


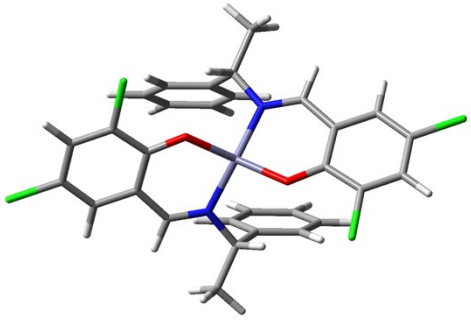
Fig. S9 Experimental and simulated ECD spectra for enantiomeric pairs (a) Zn*R*2/Zn*S*2 and (b) Zn*R*3/Zn*S*3 (*ca.* 3.00x10^{-2} mM) in methanol/chloroform (50%, v/v) at 25 °C ($\Delta\varepsilon_{exptl.}$ values are increased by 2 times). Spectra simulated at b3lyp/tzvp//b3lyp/6-31G(d) with PCM in chloroform, respectively. Gaussian band shape with exponential half-width σ = 0.16 eV.



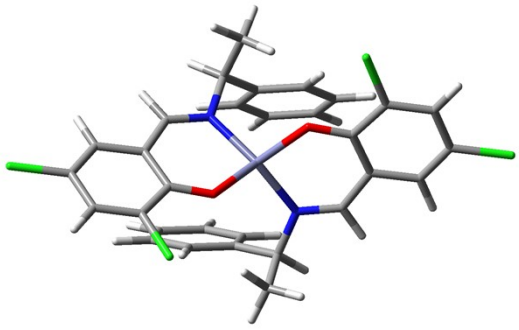
Λ-Zn*R*1, –5037.234449 a.u.; +0.99 kcal/mol



Δ-Zn*R*1, –5037.232888 a.u.



Λ-Zn*S*1, –5037.232881 a.u.



Δ-Zn*S*1, –5037.234453 a.u.; +0.99 kcal/mol

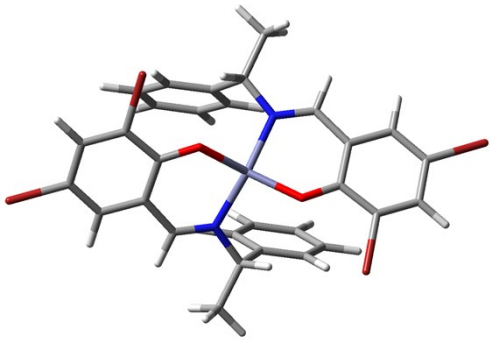
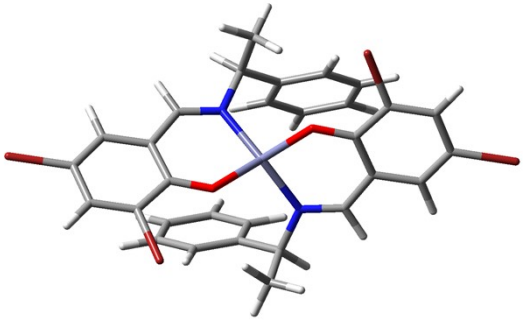
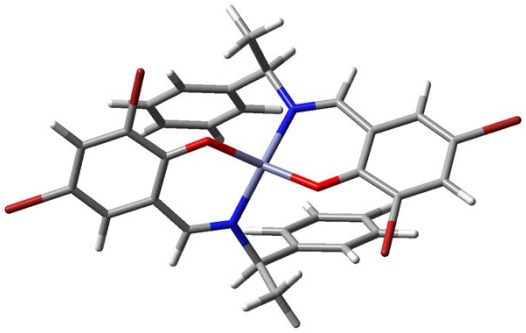
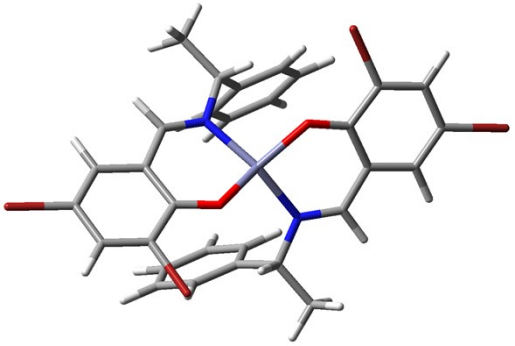
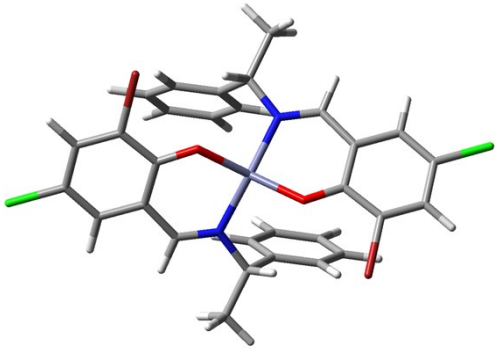
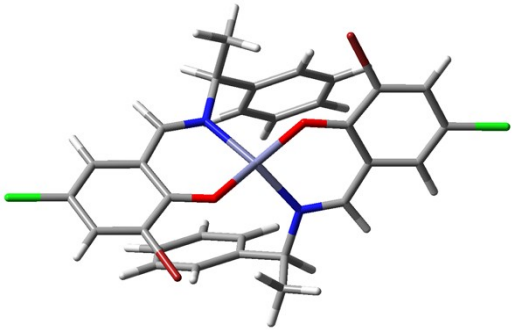
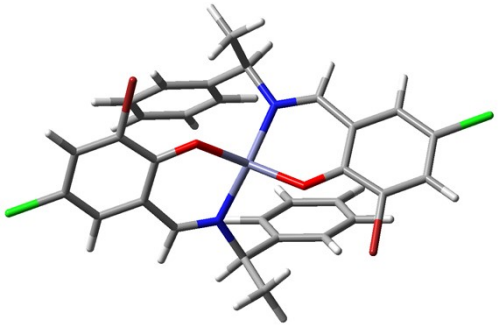
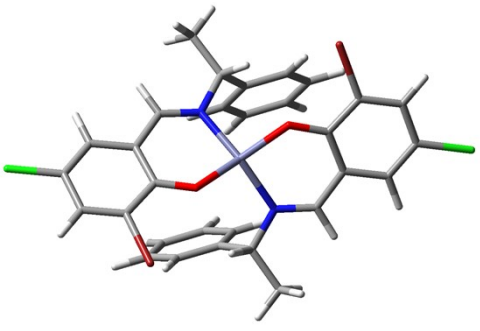
 Λ-Zn*S*2, −13483.279346 a.u.	 Δ-Zn*S*2, −13483.282278 a.u.; +1.84 kcal/mol
 Λ-Zn*R*2, −13483.282269 a.u.; +1.84 kcal/mol	 Δ-Zn*R*2, −13483.279343 a.u.
 Λ-Zn*S*3, −9260.257792 a.u.	 Δ-Zn*S*3, −9260.260826 a.u.; +1.90 kcal/mol
 Λ-Zn*R*3, −9260.260833 a.u.; +1.91 kcal/mol	 Δ-Zn*R*3, −9260.257788 a.u.

Fig. S10 Optimized structures for diastereomeric pair Λ-Zn-*R*/Δ-Zn-*R* and Δ-Zn-*S* /Λ-Zn-*S* at b3lyp/6-31g(d), respectively.

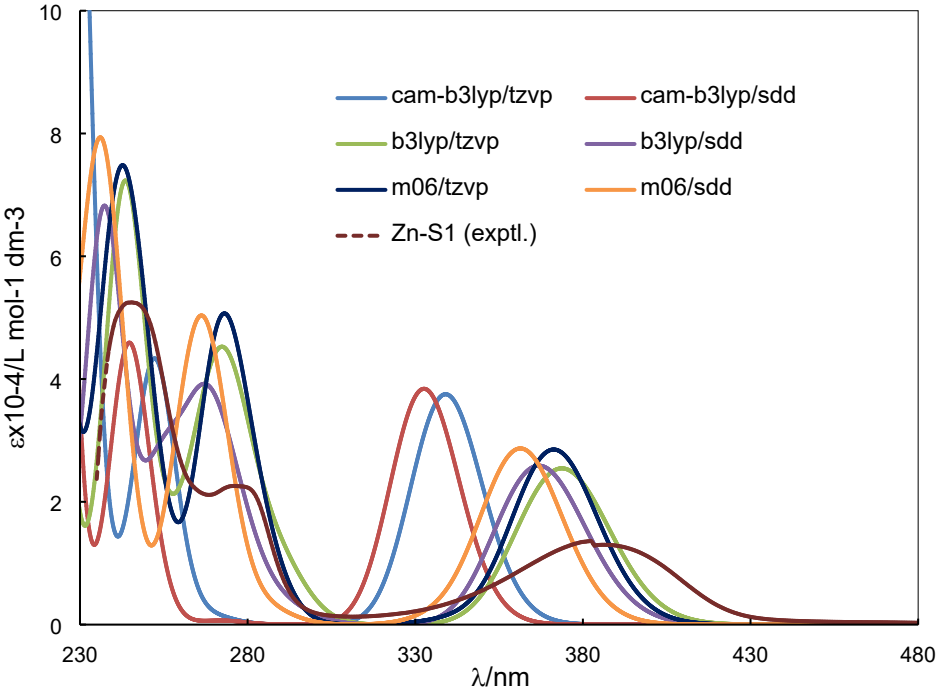


Fig. S11 Experimental UV-Vis. spectrum for Zn*S*1 (3.22x10^{-2} mM) in methanol/chloroform (50%, v/v) at 25 °C and computed UV-Vis. spectra for Δ-Zn*S*1 at different functionals and the basis sets, respectively. Gaussian band shape with exponential half-width, σ = 0.16 eV.

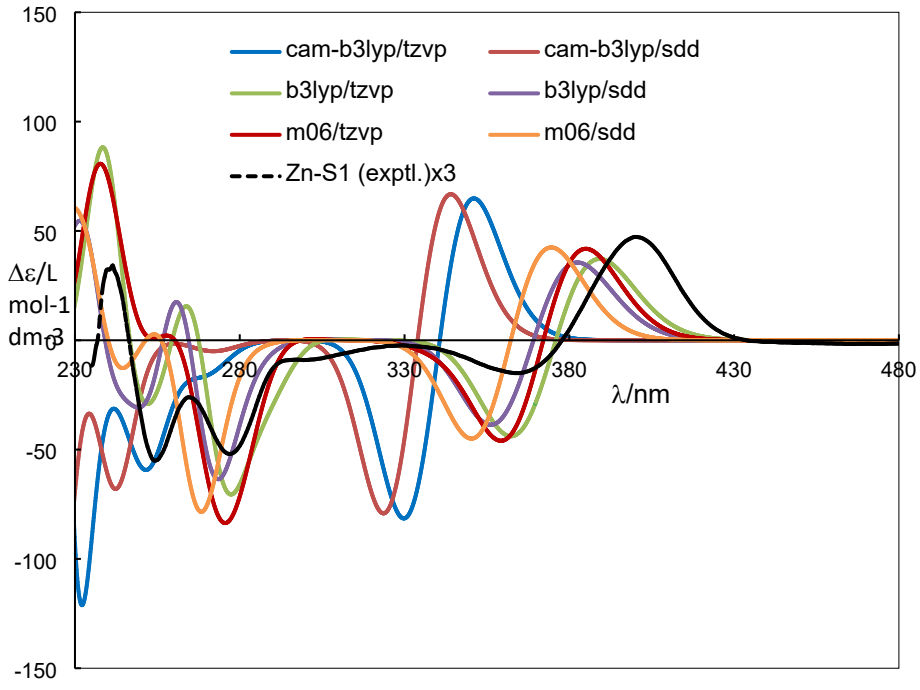


Fig. S12 Experimental ECD spectra for Zn-*S*1 (~3.00x10^{-2} mM) in methanol/chloroform (50%, v/v) at 25 °C and computed ECD spectra for Δ-Zn*S*1 at different functionals and the basis sets, respectively. Gaussian band shape with exponential half-width, σ = 0.16 eV.

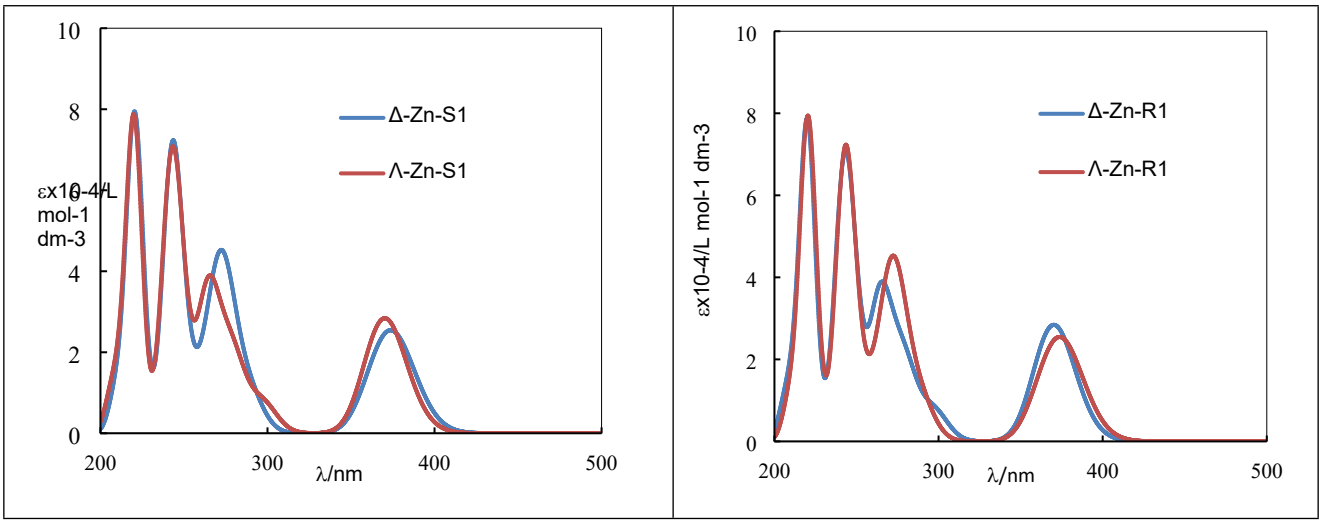
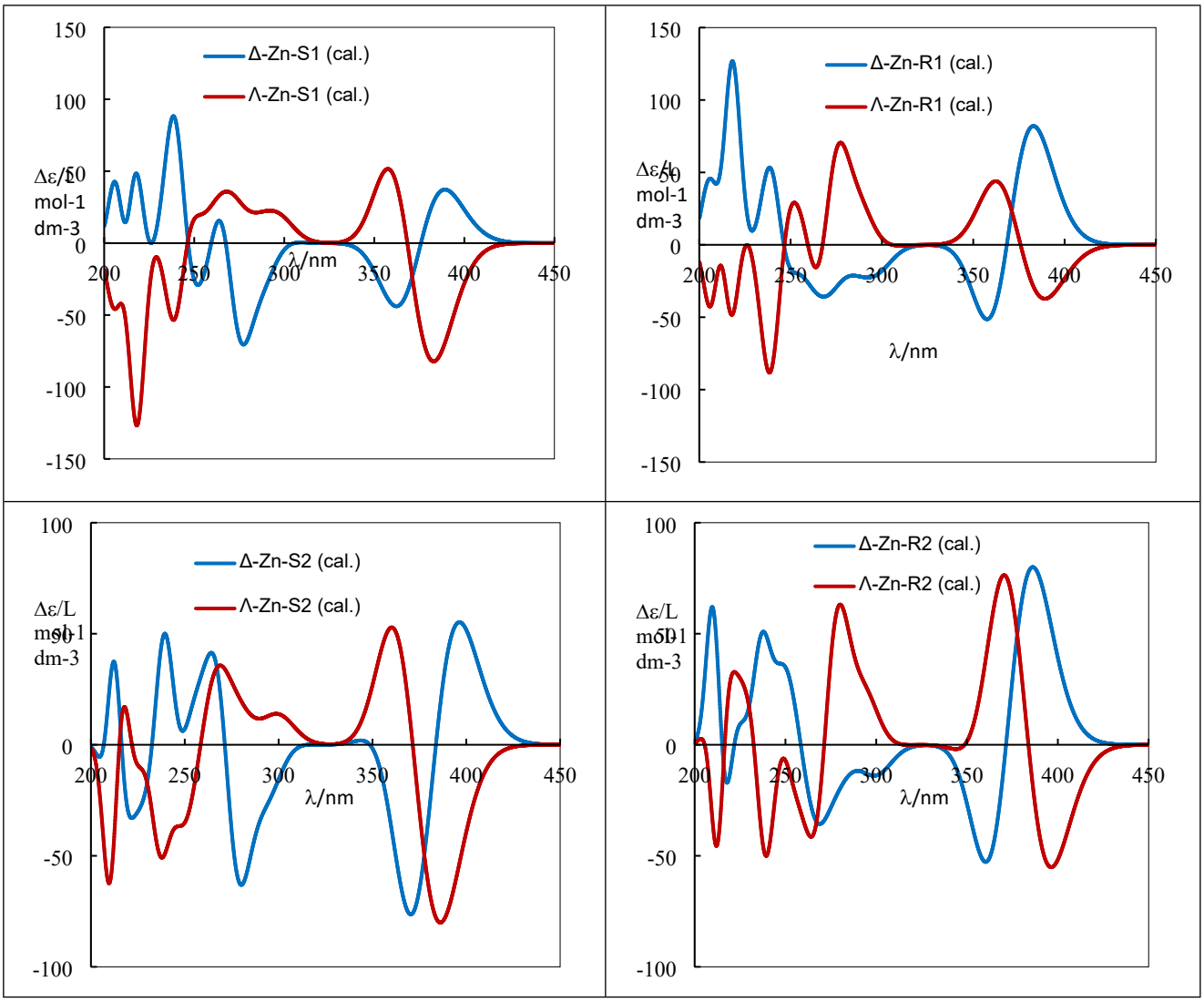


Fig. S13 Calculated UV-Vis. spectra for diastereomeric pairs Λ-Zn*S*1/Δ-Zn*S*1 and Λ-Zn*R*1/Δ-Zn*R*1 at b3lyp/tzvp//b3lyp/6-31g(d), respectively. Gaussian band shape with exponential half-width σ = 0.16 eV.



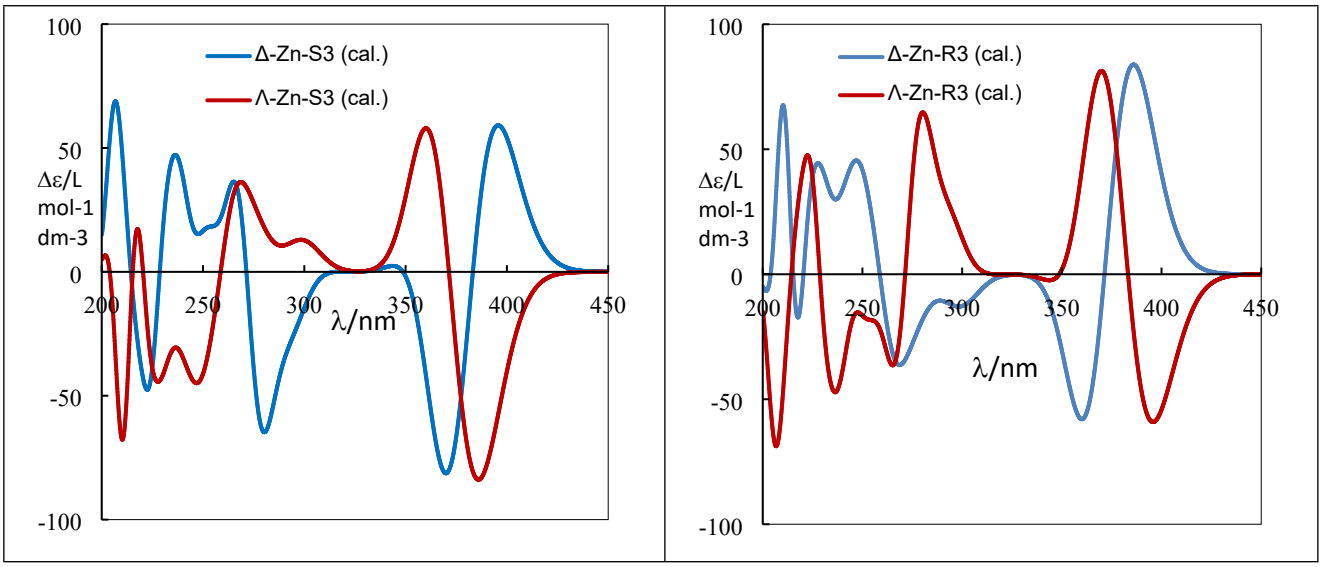
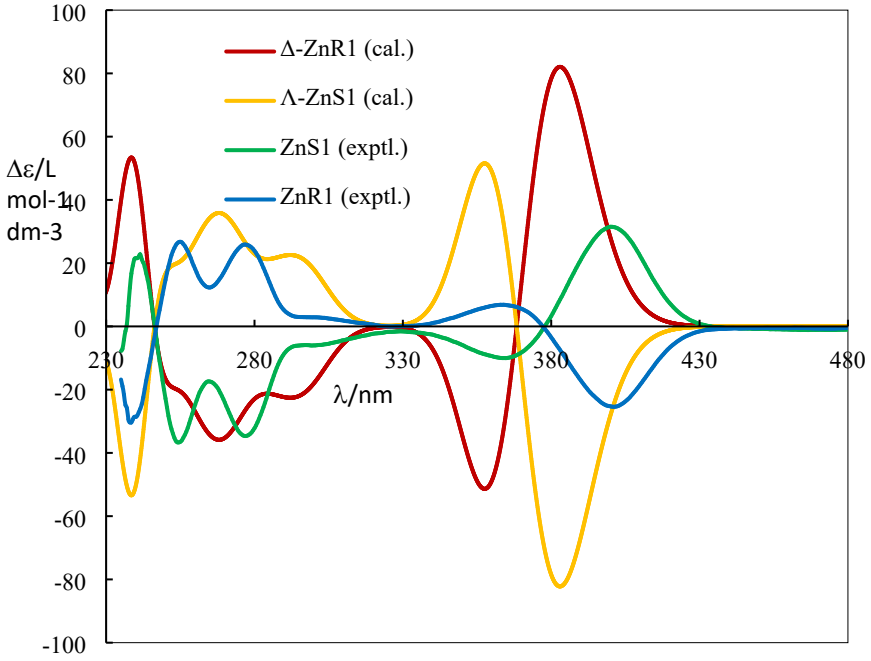


Fig. S14 Calculated ECD spectra for diastereomeric pairs Λ/Δ-Zn*S*1 and Λ/Δ-Zn*R*1; Λ/Δ-Zn*S*2 and Λ/Δ-Zn*R*2; Λ/Δ-Zn*S*3 and Λ/Δ-Zn*R*3 at b3lyp/tzvp//b3lyp/6-31g(d), respectively. Gaussian band shape with exponential half-width σ = 0.16 eV.



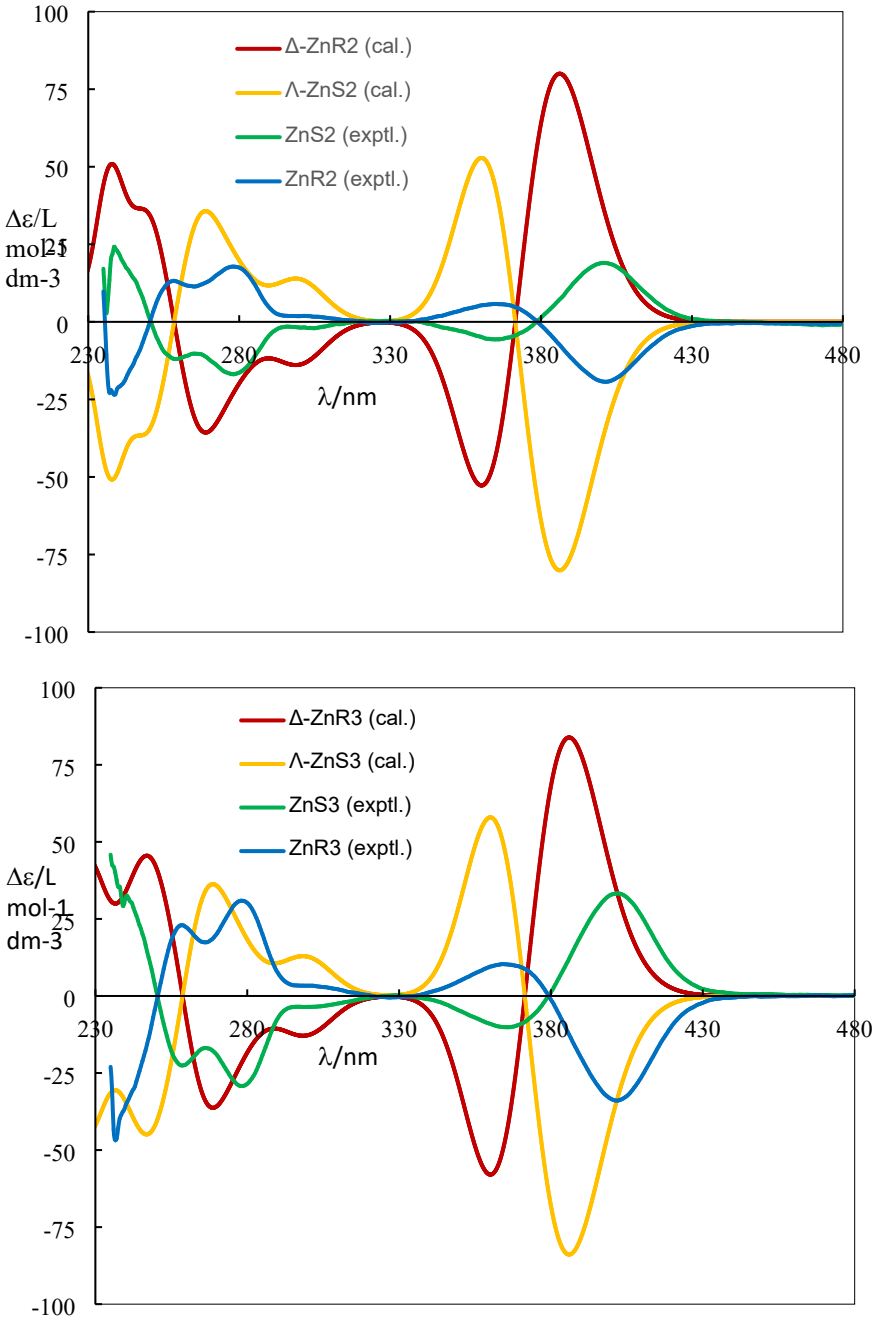


Fig. S15 Experimental and simulated ECD spectra (the opposite comparison) for Zn*R*1/Zn*S*1, Zn*R*2/Zn*S*2 and Zn*R*3/Zn*S*3 (*ca.* 3.00x10^{-2} mM) in methanol/chloroform (50%, v/v) at 25 °C ($\Delta\varepsilon_{exptl.}$ values are increased by 2 times). Spectra simulated at b3lyp/tzvp//b3lyp/6-31G(d) with PCM in chloroform, respectively. Gaussian band shape with exponential half-width σ = 0.16 eV.

Table S1. Crystal data and structure refinement for Zn(II)-*Chiral* Schiff bases complexes.

	Λ-Zn*R*1	Λ-Zn*R*2	Λ-Zn*R*3	Δ-Zn*S*1	Δ-Zn*S*2	Δ-Zn*S*3
Empirical formula	$C_{30}H_{24}Cl_4ZnN_2O_2$	$C_{30}H_{24}Br_4ZnN_2O_2$	$C_{30}H_{24}Br_2Cl_2ZnN_2O_2$	$C_{30}H_{24}Cl_4ZnN_2O_2$	$C_{30}H_{24}Br_4ZnN_2O_2$	$C_{30}H_{24}Br_2Cl_2ZnN_2O_2$
M (g mol^{-1})	651.68	829.52	740.60	651.68	829.52	740.60
Temperature (K)	160(1)	160(1)	160(1)	160(1)	160(1)	160(1)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	1.54184
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic

Space group	I2	I2	I2	I2	I2	I2
a (Å)	10.08126(12)	10.2155(3)	10.21573(14)	10.0890(3)	10.2179(3)	10.2247(2)
b (Å)	10.86962(12)	10.9297(3)	10.88240(13)	10.8821(3)	10.9275(3)	10.8940(3)
c (Å)	12.76560(16)	12.9935(3)	12.90981(18)	12.7748(3)	12.9953(4)	12.9214(3)
β (°)	106.5627(13)	106.622(3)	107.2179(14)	106.586(3)	106.617(3)	107.216(3)
V (Å^3)	1340.81(3)	1390.14(7)	1370.89(3)	1344.19(7)	1390.41(8)	1374.80(6)
$Z/D_{calc.}$(g cm^{-3})	2/ 1.614	2/ 1.982	2/1.794	2/1.610	2/1.981	2/1.789
μ (mm^{-1})	1.348	6.665	4.038	1.344	6.663	6.697
F(000)	664.0	808.0	736.0	664.0	808.0	736.0
θ range (°)	5.012 to 61.012	4.96 to 52.734	5.608 to 52.744	5.636 to 52.738	4.96 to 52.728	9.744 to 148.854
h; k; l ranges	±14; ±15; ±18	±12; ±13; -15,+16	±12; ±13; ±16	±12; ±13; ±15	±12; ±13; ±16	±12; ±13; ±16
Reflections collected	20946	14589	15540	12841	14735	8416
Independent reflect. (R_{int})	4106 (0.0211)	2841 (0.0208)	2801 (0.0223)	2754 (0.0325)	2839 (0.0411)	2762 (0.0154)
Data/restraints/parameters	4106/1/178	2841/1/178	2801/1/178	2754/1/178	2839/1/178	2762/1/178
Goodness-of-fit on F^2[a]	1.066	1.058	1.056	1.034	0.997	1.057
R_1/wR_2 [I>2σ (I)][b]	0.0189/ 0.0511	0.0134/0.0330	0.0185/0.0472	0.0238/0.0558	0.0180/0.0416	0.0222/0.0587
R_1/wR_2 (all data)[b]	0.0192/ 0.0512	0.0138/0.0332	0.0186/0.0473	0.0265/0.0572	0.0193/0.0418	0.0224/0.0589
Max./min. $\Delta\rho$ (e. Å^{-3})[c]	0.50/-0.18	0.31/-0.17	0.17/-0.21	0.45/-0.27	0.45/-0.27	0.19/-0.51
Flack parameter[d]	-0.004(3)	-0.010(4)	-0.003(8)	-0.010(6)	0.011(5)	-0.007(19)
CCDC number	2000646	2000644	2000648	2000652	2000650	2000653
Code	hadi2711	hadi1611	Hadi2111	hadi2211	hadi1511	Hadi2011

[a] Goodness-of-fit = $[\sum[w(F_o^2 - F_c^2)^2]/(n-p)]^{1/2}$; [b] $R_1=[\sum(||F_o| - |F_c||)/\sum|F_o|]$; $wR_2=[\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; [c] Largest difference peak and hole; [d] Absolute structure parameter.[1-4]

Table S2. Values of dihedral angle (θ/°) and geometric indexes ($\tau_{tet\text{-}sq}$ and τ_4) in the Zn(II)-*chiral* Schiff base complexes.

Entity	X_1, X_2	θ/°	$\tau_{tet\text{-}sq}$[a]	τ_4[b]
Λ-Zn*R*1	Cl, Cl	75.93	0.84	0.75
Δ-Zn*S*1	Cl, Cl	76.14	0.85	0.75
Λ-Zn*R*2	Br, Br	75.92	0.84	0.75
Δ-Zn*S*2	Br,Br	76.10	0.85	0.75
Λ-Zn*R*3	ClBr	75.46	0.84 0.84	0.75
Δ-Zn*S*3	ClBr	75.47		0.75

[a] $\tau_{tet\text{-}sq} = \theta/90$. [b] $\tau_4 = [\{360° - (\alpha + \beta)\}/141]°$, where α, β are the two largest angles in Table 1. Note: θ should be 90° for a tetrahedral geometry and 0° for a square planar geometry (not considering the imminent distortion induced by the chelate ring formation).[51] Accordingly $\tau_{tet\text{-}sq}$ = 1.00 for tetrahedral and 0.00 for square planar geometry. τ_4 = 1.00 for a perfect tetrahedral geometry and 0.00 for a perfect square planar geometry.[52] For two chelate ligands, as in the present bis-bidentate Schiff base complexes, τ_4 will not correctly assess a tetrahedral geometry because of the already imminent distortion induced by the chelate ring formation.

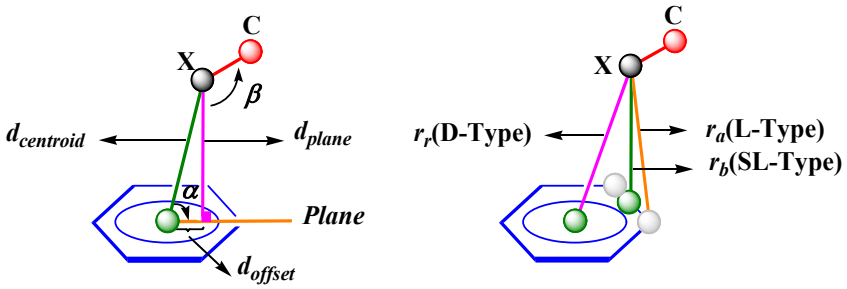
Table S3. Supramolecular X…O(1) interactions in Zn(II)-complexes.

Entity	X =	X···O(1)/Å	C(4)—X···O(1)/°	C(1)—O(1)···X/°	< or > normal X···O bond (%)

Λ-Zn-*R*1	Cl(2)	3.402	141.220	143.575	+ 1.85
Δ-Zn-*S*1	Cl(2)	3.407	141.210	143.677	+ 2.00
Λ-Zn-*R*2	Br(2)	3.342	141.265	143.069	- 3.13
Δ-Zn-*S*2	Br(2)	3.345	141.234	143.056	- 3.04
Λ-Zn-*R*3	Cl(1)	3.431	140.984	143.062	+ 2.72
Δ-Zn-*S*3	Cl(1)	3.433	141.163	143.404	+ 2.78

Table S4. Geometrical parameters (Å and °) for descriptions of C–X···π interactions in Zn(II)-complexes.

Definition of geometrical C–X···π parameters



	Λ-Zn*R*1/Δ-Zn*S*1	Λ-Zn*R*2/Δ-Zn*S*2	Λ-Zn*R*3/Δ-Zn*S*3
C–X···π[1]	C–Cl_1···π	C–Br_1···π	C–Br_1···π
r_r/ Å	3.883/3.885	3.806/3.807	3.790/3.793
r_a/ Å	3.523/3.527 (C9)	3.473/3.473 (C9)	3.454 (C14)/3.463 (C10)
r_b/ Å	3.472/3.474	3.404/3.404	3.390/3.395
D_{plane}/ Å	3.402/3.404	3.341/3.342	3.333/3.337
$d_{centroid}$/ Å	3.883/3.885	3.806/3.807	3.790/3.793
d_{offset}/ Å	1.872/1.871	1.823/1.822	1.805/1.803
α/ °	61.17/61.21	61.38/61.41	61.56/61.61
β/ °	145.18/144.97	145.64/145.66	146.16/146.18
Type	SL	SL	SL

[1] π (C_9-C_{14}).

Analysis of intra-molecular interactions for the Δ-Zn*S*/Λ-Zn*S*, resp. Λ-Zn*R*/Δ-Zn*R* diastereomeric difference.

Table S5. 70 Strongest inter-fragment interactions as IBSIW index for Δ-Zn*S*1.

atom # Frag1	atom # Frag2 [a]	IBSIW index [a.u./Å^2]	Interaction
27	63	1.558382	(CH3)C-H...O
31	59	1.557899	O...H-C(CH3)
15	33	0.997136	(Ph)C-H...C(sal)
1	47	0.996316	(sal)C...H-C(Ph)
15	63	0.906876	(Ph)C-H...O
31	47	0.905773	O...H-C(Ph)
31	62	0.623283	O...N
30	63	0.623207	N...O
28	59	0.448733	Cl...H-C(CH3)
27	60	0.448715	(CH3)C-H...Cl
1	46	0.445425	(sal)C...C(Ph)
14	33	0.445102	(Ph)C...C(sal)
31	46	0.429735	O...C(Ph)
14	63	0.429632	(Ph)C...O
31	56	0.418336	O...C(CH3)
24	63	0.418314	(CH3)C...O
21	53	0.371012	(Ph)C-H...H-C(Ph)
2	47	0.350234	(sal)C...H-C(PH)
15	34	0.350018	(Ph)C-H...C(sal)
27	33	0.345781	(CH3)C-H...C(sal)
1	59	0.345639	(sal)C...H-C(CH3)
20	52	0.321164	(Ph)C...C(Ph)
15	40	0.302054	(Ph)C-H...C(sal)
8	47	0.301647	(sal)C...H-C(Ph)
31	63	0.296042	O...O
22	52	0.293353	(Ph)C...C(Ph)
20	54	0.293054	(Ph)C...C(Ph)
31	43	0.289533	O...C(C-methin)
11	63	0.289405	(methin-C)C...O
22	54	0.261365	(Ph)C...C(Ph)
8	46	0.255609	(sal)C...C(Ph)
14	40	0.255479	(Ph)C...C(sal)
20	53	0.254196	(Ph)C...H-C(Ph)
21	52	0.253586	(Ph)C-H...C(Ph)
20	55	0.222963	(Ph)C...H-C(Ph)
23	52	0.222903	(Ph)C-H...C(Ph)
30	62	0.200424	N...N
14	41	0.183581	(Ph)C...C(imin)
9	46	0.183569	(imin)C...C(Ph)
31	45	0.175972	O...C(Ph)
13	63	0.175729	(Ph)C...O
28	47	0.160912	Cl...H-C(Ph)
15	60	0.160718	(Ph)C-H...Cl
8	48	0.155667	(sal)C...C(Ph)
16	40	0.155500	(Ph)C...C(sal)
18	55	0.154467	(Ph)C...H-C(Ph)
23	50	0.154166	(Ph)C-H...C(Ph)
2	59	0.153368	(sal)C...C(CH3)
27	34	0.153359	(CH3)C-H...C(sal)
14	62	0.142815	(Ph)C...N
30	46	0.142657	N...C(Ph)

9 48	0.132594	(imin)C...C(Ph)
16 41	0.132553	(Ph)C...C(imin)
22 53	0.121706	(Ph)C...H-C(Ph)
21 54	0.121308	(Ph)C-H...C(Ph)
8 49	0.116124	(sal)C...H-C(Ph)
17 40	0.116070	(Ph)C-H...C(sal)
1 48	0.113776	(sal)C...C(Ph)
16 33	0.113625	(Ph)C...C(sal)
18 54	0.106890	(Ph)C...C(Ph)
22 50	0.106832	(Ph)C...C(Ph)
30 45	0.105881	N...C(Ph)
13 62	0.105762	(Ph)C...N
2 46	0.104529	(sal)C...C(Ph)
14 34	0.104384	(Ph)C...C(sal)
15 41	0.103609	(Ph)C-H...C(imin)
9 47	0.103389	(imin)C...H-C(Ph)
22 55	0.102645	(Ph)C...H-C(Ph)
23 54	0.102522	(Ph)C-H...C(Ph)
28 56	0.098306	Cl...C(CH3)
SUM	**22.09**	

[a] Fragment 1 is the ligand with atom numbers 1-31, fragment 2 the ligand with atom numbers 33-63. For atom numbering see the following graph:

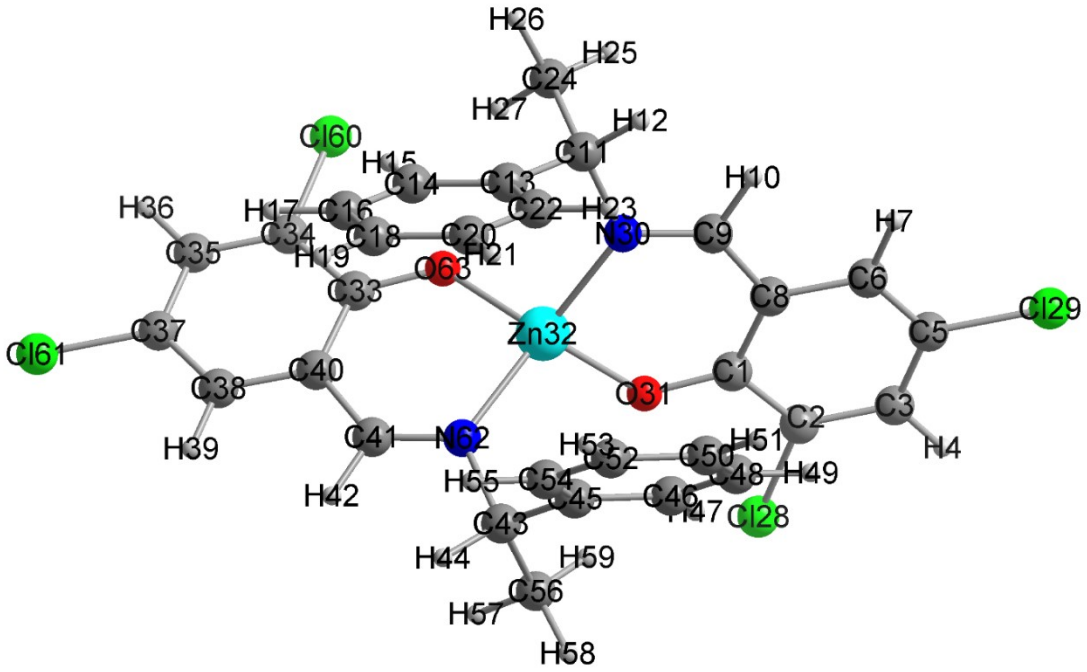


Table S6. 70 Strongest inter-fragment interactions as IBSIW index for Λ-Zn*S*1.

atom # Frag1 atom # Frag2 [a]	IBSIW index [a.u./Å²]	Interaction
12 63	1.635349	(methin)C-H...O
31 44	1.634854	O...H-C(methin)
30 63	0.861119	N...O
31 62	0.860700	O...N
11 63	0.699037	(methin)C...O
31 43	0.698832	O...C(methin)
21 53	0.490237	(Ph)C-H...H-C(Ph)
20 52	0.463831	(Ph)C...C(Ph)
21 52	0.405366	(Ph)C-H...C(Ph)
20 53	0.405207	(Ph)C...H-C(Ph)

1 47	0.392874	(sal)C...H-C(Ph)
15 33	0.392374	(Ph)C-H...C(sal)
12 33	0.349622	(methin)C-H...C(sal)
1 44	0.349489	(sal)C...H-C(methin)
31 47	0.267812	O...H-C(Ph)
15 63	0.267390	(Ph)C-H...O
2 47	0.256915	(sal)C...H-C(Ph)
15 34	0.256768	(Ph)C-H...C(sal)
12 60	0.251530	(methin)C-H...Cl
28 44	0.251474	Cl...H-C(methin)
1 46	0.240414	(sal)C...C(Ph)
14 33	0.240302	(Ph)C...C(sal)
20 54	0.226918	(Ph)C...C(Ph)
22 52	0.226912	(Ph)C...C(Ph)
31 63	0.212265	O...O
13 63	0.205910	(Ph)C...O
31 45	0.205861	O...C(Ph)
22 54	0.202005	(Ph)C...C(Ph)
31 46	0.197169	O...C(Ph)
14 63	0.197005	(Ph)C...O
28 47	0.189200	(Ph)C-H...Cl
15 60	0.189046	Cl...H-C(Ph)
30 62	0.171955	N...N
11 33	0.150363	(methin)C...C(sal)
1 43	0.150317	(sal)C...C(methin)
21 50	0.146598	(Ph)C-H...C(Ph)
18 53	0.146473	(Ph)C...H-C(Ph)
23 52	0.120439	(Ph)C-H...C(Ph)
20 55	0.120400	(Ph)C...H-C(Ph)
12 34	0.117854	(methin)C-H...C(sal)
2 44	0.117782	(sal)C...H-C(methin)
20 50	0.113147	(Ph)C...C(Ph)
18 52	0.113082	(Ph)C...C(Ph)
13 33	0.111814	(Ph)C...C(sal)
1 45	0.111773	(sal)C...C(Ph)
30 33	0.104050	N...C(sal)
1 62	0.104023	(sal)C...N
14 40	0.103307	(sal)C...C(Ph)
8 46	0.103301	(Ph)C...C(sal)
8 47	0.101304	(sal)C...H-C(Ph)
15 40	0.101225	(Ph)C-H...C(sal)
21 54	0.095149	(Ph)C-H...C(Ph)
22 53	0.095104	(Ph)C...H-C(Ph)
23 50	0.094665	(Ph)C-H...C(Ph)
18 55	0.094569	(Ph)C...H-C(Ph)
22 50	0.089953	(Ph)C...C(Ph)
18 54	0.089914	(Ph)C...C(Ph)
2 46	0.088889	(Ph)C...C(sal)
14 34	0.088872	(sal)C...C(Ph)
9 63	0.086210	(imin)C...O
31 41	0.086188	O...C(sal)
23 54	0.077541	(Ph)C-H...C(Ph)
22 55	0.077529	(Ph)C...H-C(Ph)
22 45	0.071673	(Ph)C...C(Ph)
13 54	0.071616	(Ph)C...C(Ph)
21 51	0.070256	(Ph)C-H...H-C(Ph)
19 53	0.070212	(Ph)C-H...H-C(Ph)
13 62	0.061649	(Ph)C...N
30 45	0.061640	N...C(Ph)

3 47	0.054666	(sal)C...H-C(Ph)
Sum	**17.56**	

[a] Fragment 1 is the ligand with atom numbers 1-31, fragment 2 the ligand with atom numbers 33-63. For atom numbering see the following graph:

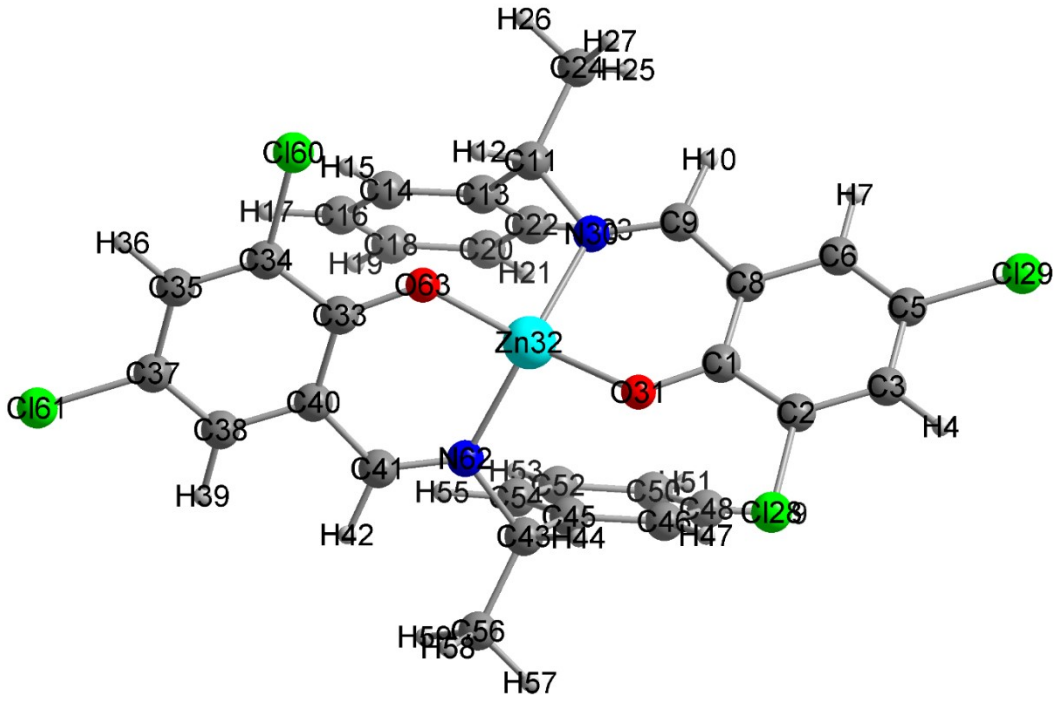


Table S7. Sum of related IBSIW indices for each atom in the fragments in the Δ-Zn*S*1 and Λ-Zn*S*1 diastereomers and the largest differences between Δ-Zn*S*1 and Λ-Zn*S*1.

	Δ-Zn*S*1		Λ-Zn*S*1		
atom # in Frag1, Frag2 [a]	Frag 1 IBSIW [a.u./Å^2]	Frag 2 IBSIW [a.u./Å^2]	Frag 1 IBSIW [a.u./Å^2]	Frag2 IBSIW [a.u./Å^2]	difference Δ-Zn*S*1 – Λ-Zn*S*1 [b]
O 31, 63	5.016727	5.017636	4.312783	4.313428	0.70
(Ph)H 15, 47	3.067974	3.065524	1.371806	1.373200	1.70
(CH3)H 27, 59	2.587759	2.587120	0.018957	0.006196	2.57
(sal)C 1, 33	2.433725	2.433980	1.500074	1.499688	0.93
(Ph)C 14, 46	1.855479	1.855743	0.935916	0.936427	0.92
N 30, 62	1.497890	1.497993	1.457919	1.457443	
(Ph)C 20, 52	1.288187	1.288282	1.462662	1.462719	
(Ph)C 22, 54	1.184627	1.184643	0.946608	0.946410	
(sal)C 8, 40	1.025359	1.025272	0.428478	0.428454	0.60
(Ph)H, 21, 53	0.919401	0.920912	1.286846	1.286424	
(Ph)C 13, 45	0.859861	0.859959	0.754145	0.754100	
Cl 28, 60	0.832169	0.831889	0.601851	0.601769	
(Ph)C 16, 48	0.817376	0.817564	0.307468	0.307693	0.51
(Ph)H 23, 55	0.782842	0.783780	0.532347	0.531955	

(imin)C 9, 41	0.780965	0.781015	0.354005	0.353962	
(sal)C 2, 34	0.760858	0.760285	0.570532	0.570474	
(CH3)C 24, 56	0.689197	0.689216	0.060345	0.060316	0.63
(methin)C 11, 43	0.602369	0.602475	1.102581	1.102276	–0.50
(Ph)C 18, 50	0.513108	0.512874	0.508766	0.509105	
(Ph)H 17, 49	0.491622	0.491852	0.090505	0.090587	
(sal)C 6, 38	0.250039	0.249909	0.079437	0.079421	
(sal)C 3, 35	0.139626	0.139509	0.101795	0.101775	
(Ph)H 19, 51	0.118323	0.118299	0.157192	0.157271	
(imin)H 10, 42	0.105191	0.105189	0.028772	0.028770	
(sal)C 5, 37	0.099346	0.099244	0.043575	0.043571	
(CH3)H 25, 57	0.096290	0.096227	0.006196	0.016851	
(CH3)H 26, 58	0.089178	0.089185	0.016861	0.018938	
(methin)H 12, 44	0.062414	0.062402	2.468030	2.467230	–2.41
(sal)H 7, 39	0.051562	0.051522	0.010741	0.010739	
(sal)H 4, 36	0.015974	0.015954	0.014845	0.014846	
Cl 29, 61	0.007498	0.007484	0.002483	0.002483	
SUM (column)	29.04	29.04	21.53	21.53	5.65
		difference: 29.04 – 21.53 = 7.51			

[a] Fragment 1 is the ligand with atom numbers 1-31, fragment 2 the ligand with atom numbers 33-63. See the graphs to Table S5 and Table S6 for atom numbering.

[b] Rounded values and average from the differences between the Fragments 1 and the Fragments 2, respectively.

Table S8. Selected inter-fragment interactions as IBSIW index with the largest differences between Δ-Zn*S*1 and Λ-Zn*S*1 (cf. Table S7).[a]

a)

atom # 15 (resp. atom # 47) in Δ-Zn*S*1			atom # 15 (resp. atom # 47) in Λ-Zn*S*1		
15 33	0.997136	(Ph)C-H...C(sal)	15 33	0.392374	(Ph)C-H...C(sal)
15 63	0.906876	(Ph)C-H...O	15 63	0.267390	(Ph)C-H...O
15 34	0.350018	(Ph)C-H...C(sal)	15 34	0.256768	(Ph)C-H...C(sal)
15 40	0.302054	(Ph)C-H...C(sal)	15 60	0.189046	(Ph)C-H...Cl
15 60	0.160718	(Ph)C-H...Cl	15 40	0.101225	(Ph)C-H...C(sal)
15 41	0.103609	(Ph)C-H...C(imin)			
Sum	2.82		Sum	1.21	

b)

atom # 1 (resp. atom # 33) in Δ-Zn*S*1			atom # 15 (resp. atom # 33) in Λ-Zn*S*1		
1 47	0.996316	(sal)C...H-C(Ph)	1 47	0.392874	(sal)C...H-C(Ph)
1 46	0.445425	(sal)C...C(Ph)	1 44	0.349489	(sal)C...H-C(methin)
1 59	0.345639	(sal)C...H-C(CH3)	1 46	0.240414	(sal)C...C(Ph)

1 48	0.113776	(sal)C...C(Ph)	1 43	0.150317	(sal)C...C(methin)
			1 45	0.111773	(sal)C...C(Ph)
			1 62	0.104023	(sal)C...N
Sum	2.82		Sum	1.35	

c)

atom # 14 (resp. atom # 46) in Δ-Zn*S*1			atom # 14 (resp. atom # 46) in Λ-Zn*S*1		
14 33	0.445102	(Ph)C...C(sal)	14 33	0.240302	(Ph)C...C(sal)
14 63	0.429632	(Ph)C...O	14 63	0.197005	(Ph)C...O
14 40	0.255479	(Ph)C...C(sal)	14 40	0.103307	(Ph)C...C(sal)
14 41	0.183581	(Ph)C...C(imin)	14 34	0.088872	(Ph)C...C(sal)
14 62	0.142815	(Ph)C...N			
Sum	1.46		Sum	0.63	

[a] Listed are the inter-atom interaction between the two ligand fragments from the 70 strongest interactions (highest IBSIW indices) in Table S5 for Δ-Zn*S*1 and Table S6 for Λ-Zn*S*1. See the graphs to Table S5 and Table S6 for atom numbering.

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