Electronic Supplementary Material (ESI) for CrystEngComm.
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Electronic supplementary information (ESI)

Experimental and computational studies on pseudotetrahedral nickel(II)-(*R* or *S*)-dihalogen-salicylaldiminates with Δ- or Λ-chirality induction at-metal

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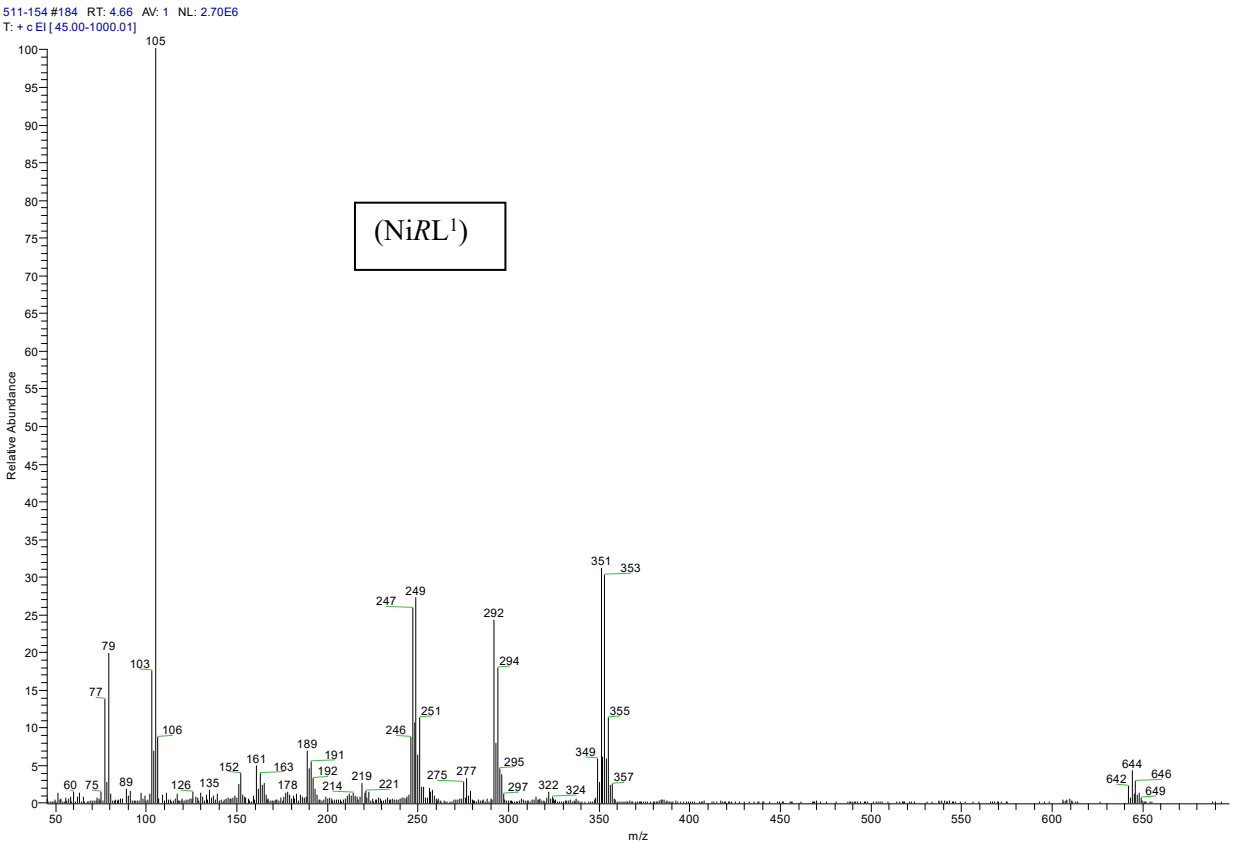

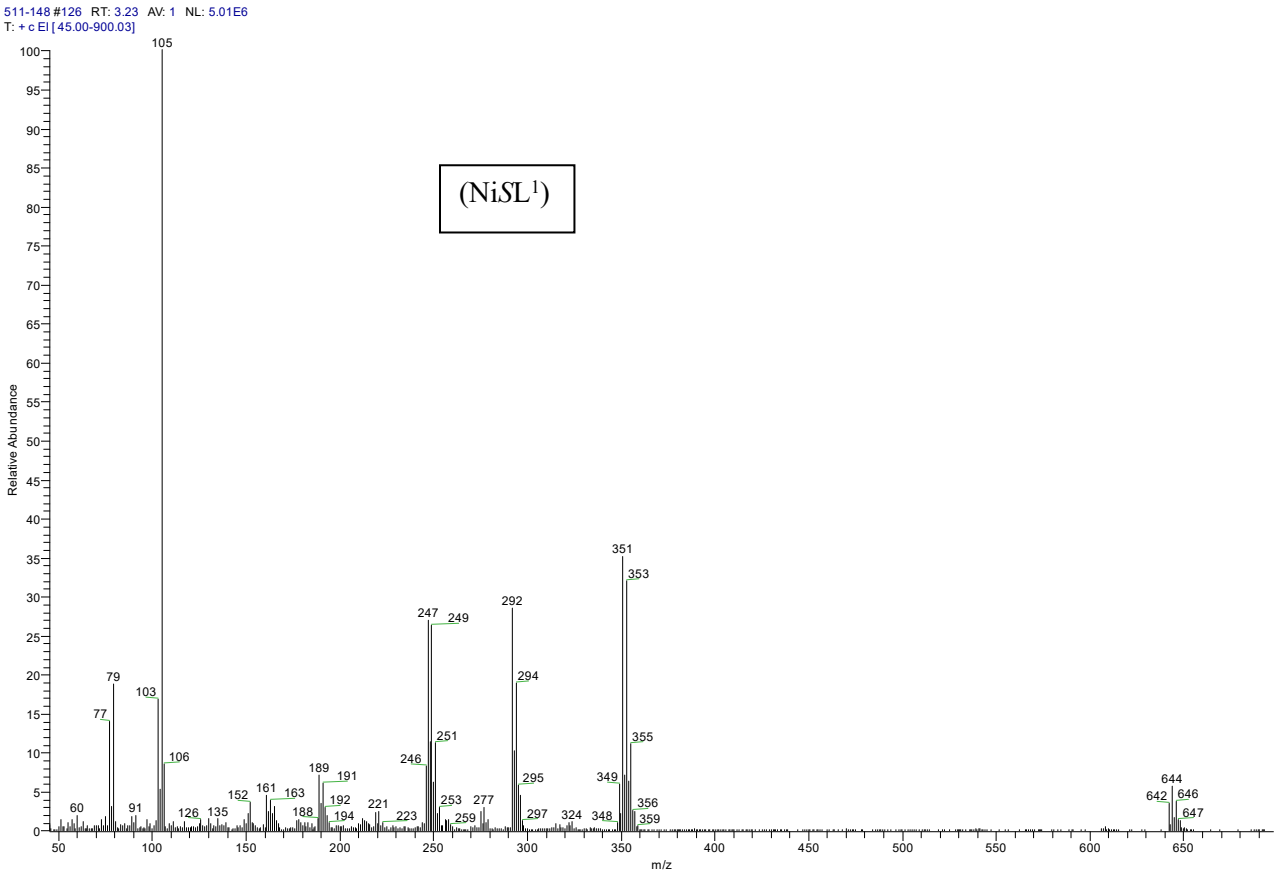
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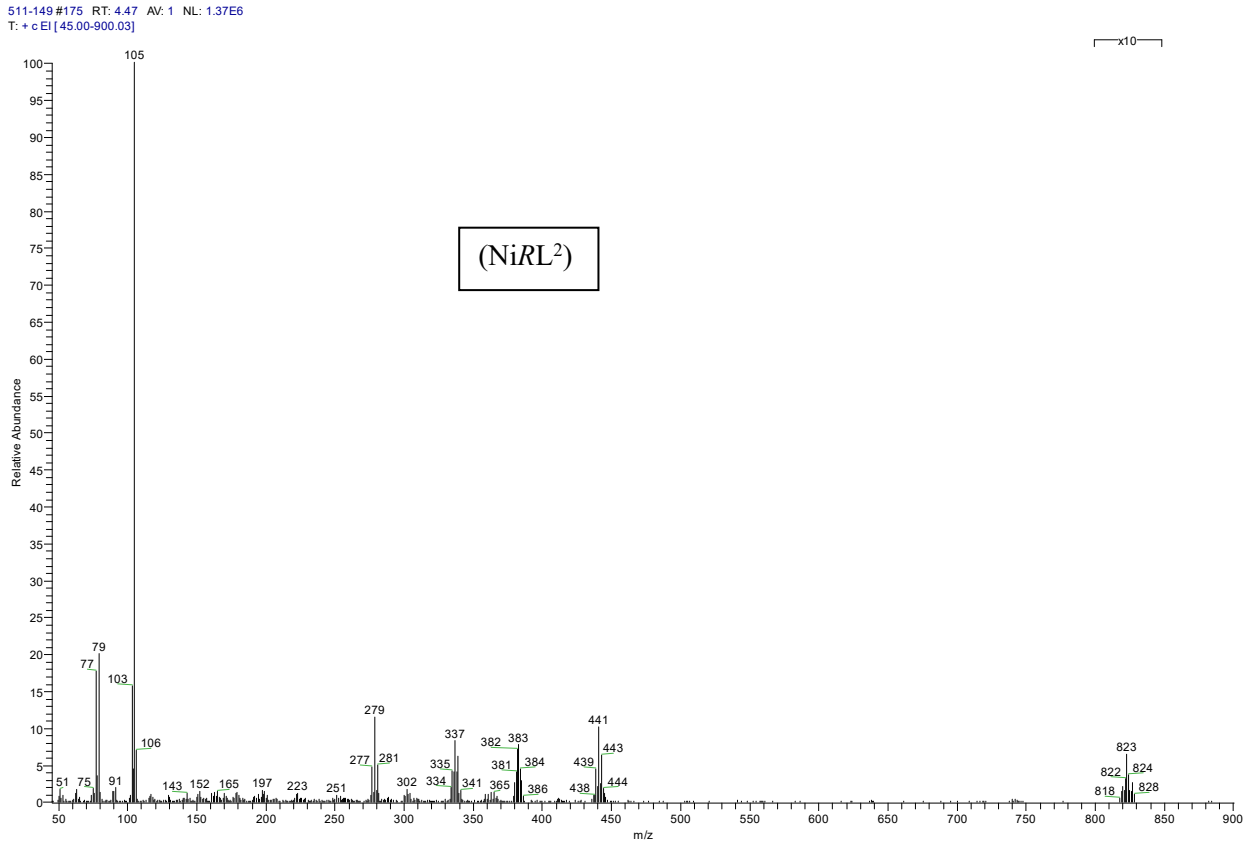
m/z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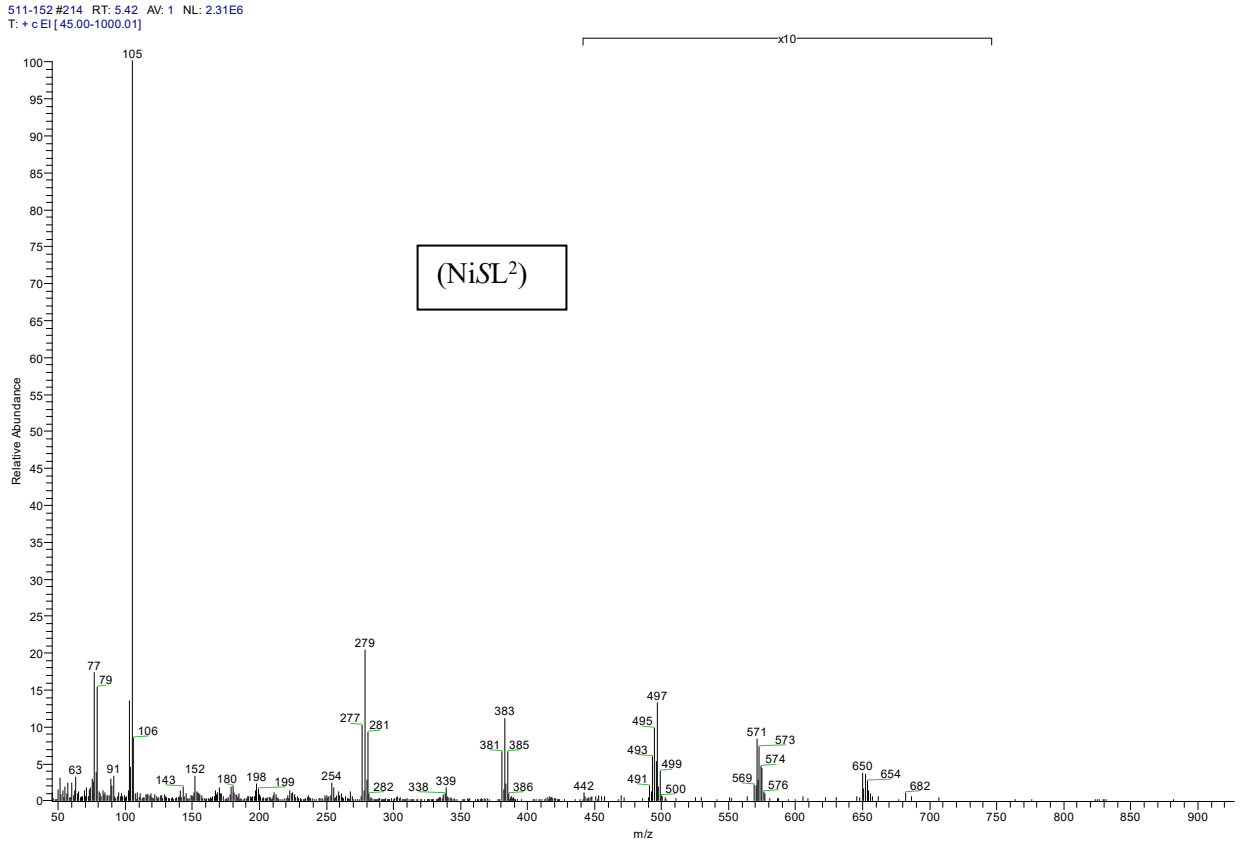
Relative Abundance
m/z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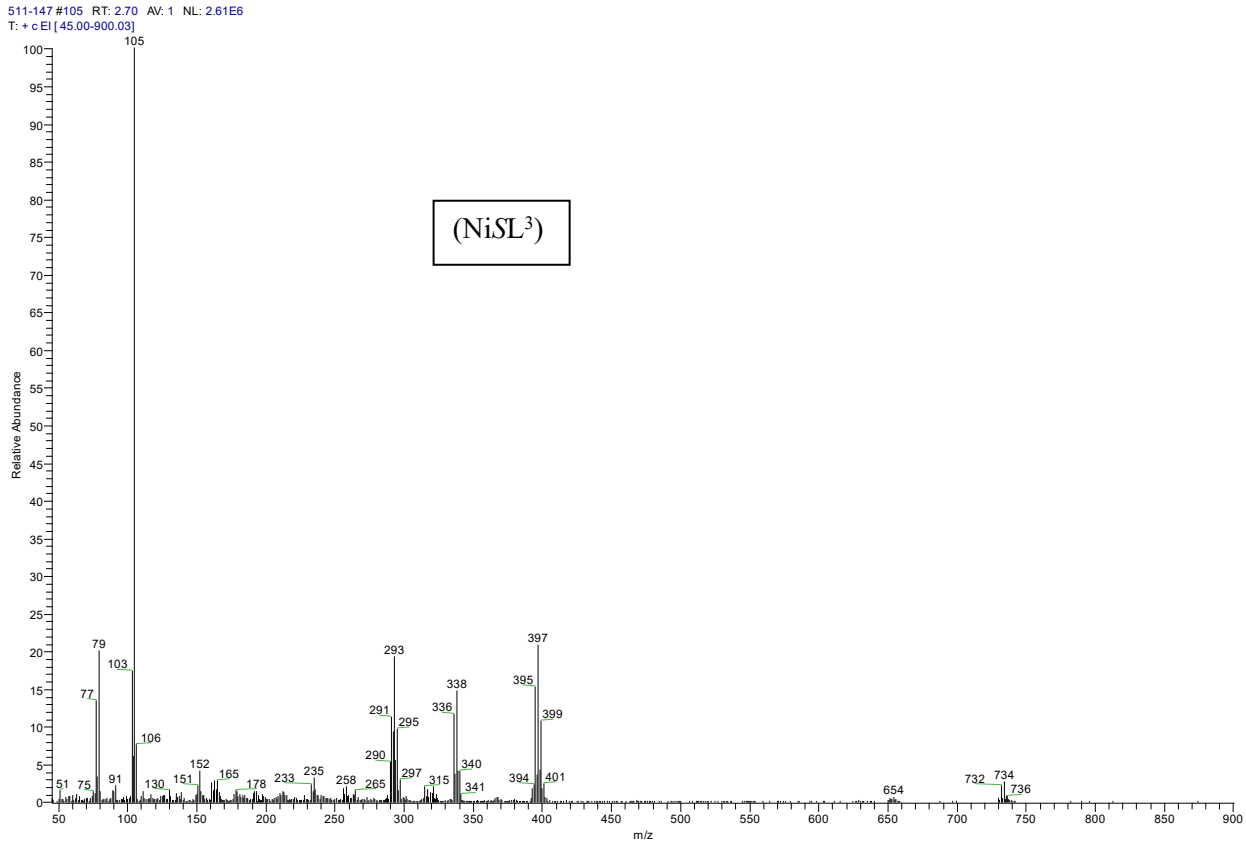
m/z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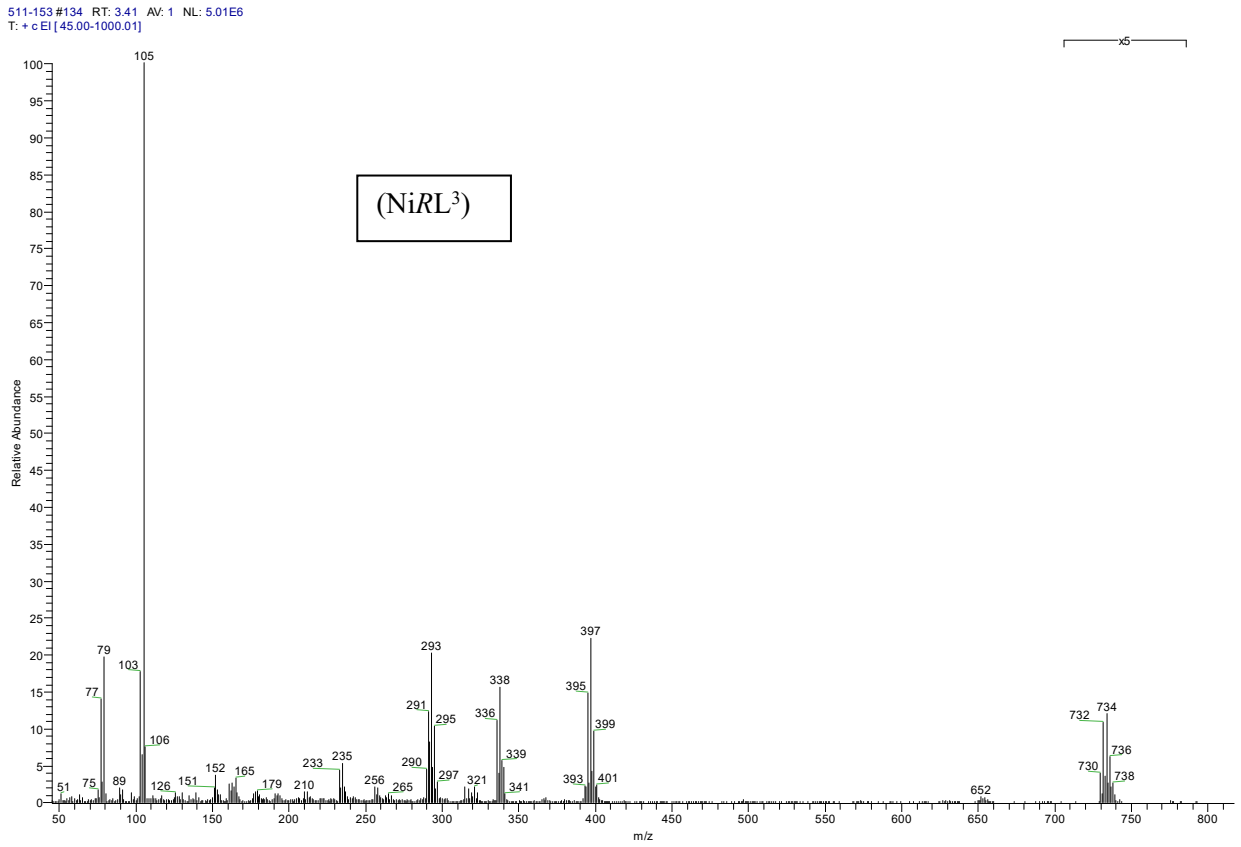
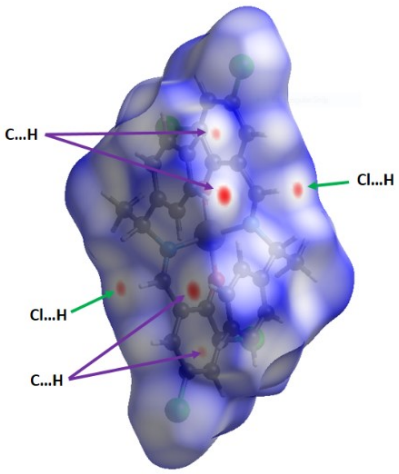
m/z

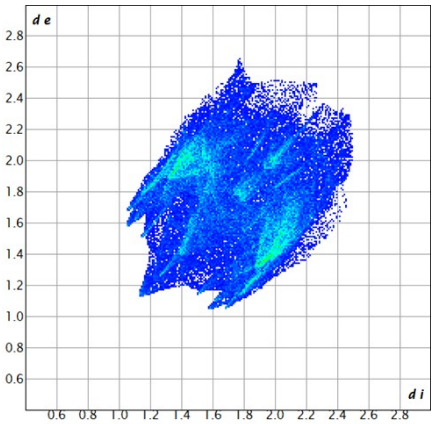


Fi

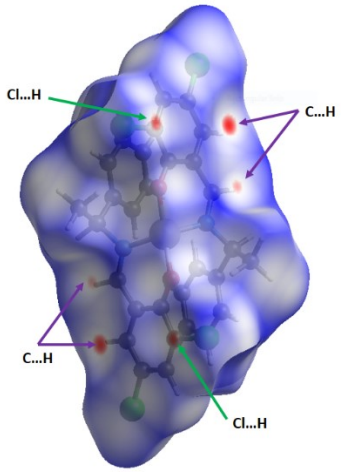
g. S1 EI-mass spectra for nickel(II)-Schiff bases complexes.

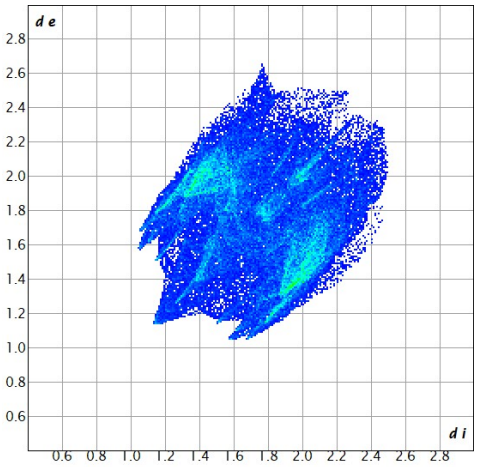
Λ-Ni*R*L^1



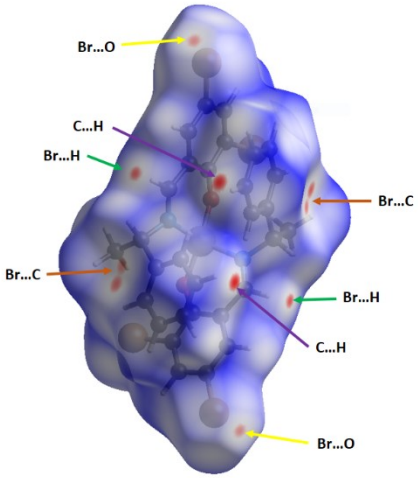


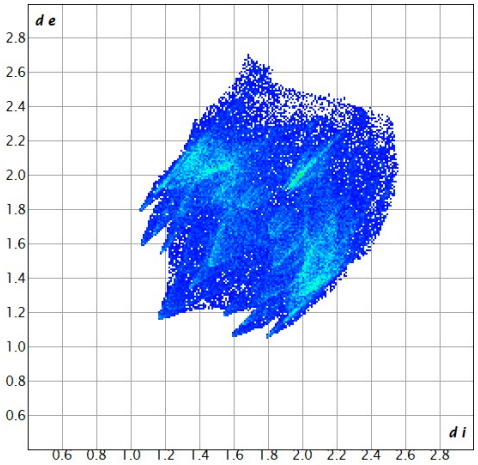
Δ-Ni*S*L^1



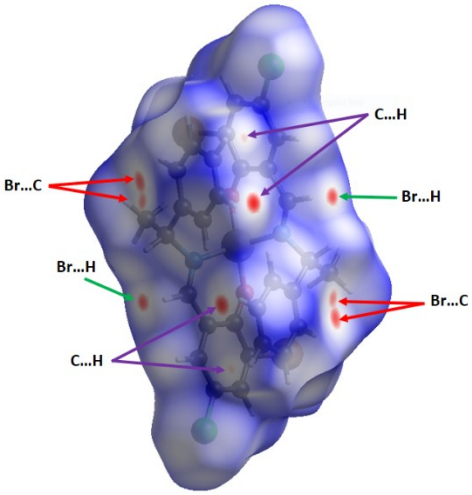


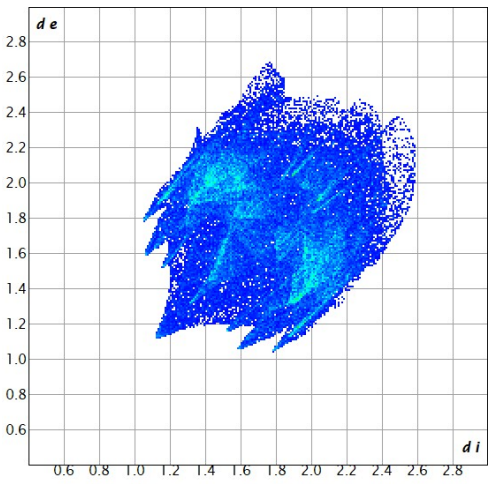
Δ-Ni*S*L²





Λ-Ni*R*L³





Δ-Ni*S*L³

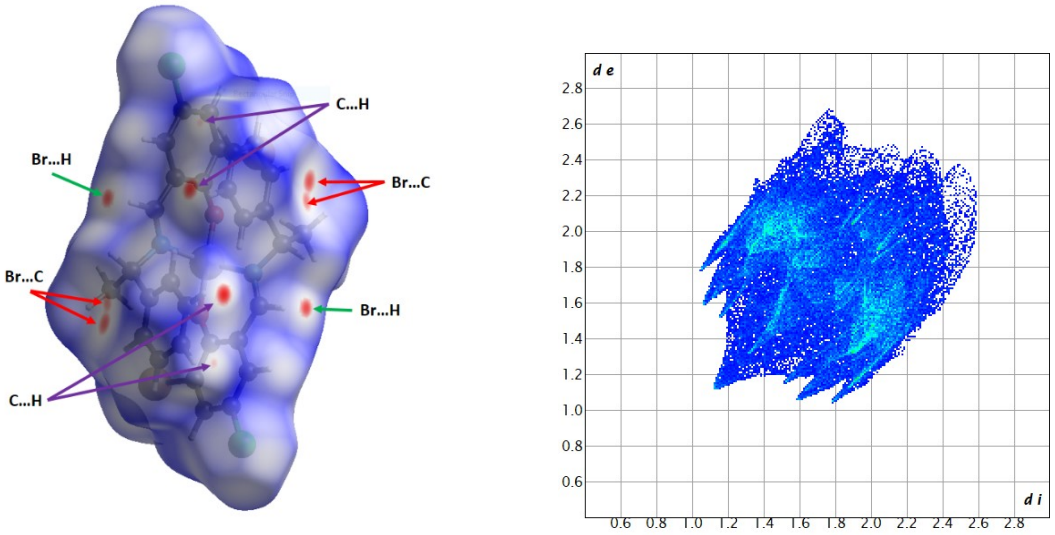


Fig. S2 Hirshfeld surfaces mapped with d_{norm} properties and fingerprint plots for Λ-Ni*R*L[1,3] and Δ-Ni*S*L[1-3]. Red spots represent the closest contacts and blue the most distant contacts. ESP (Electrostatic potential) plotted on Hirshfeld surface mapped from –0.875 au (red) to 1.1415 au (blue).

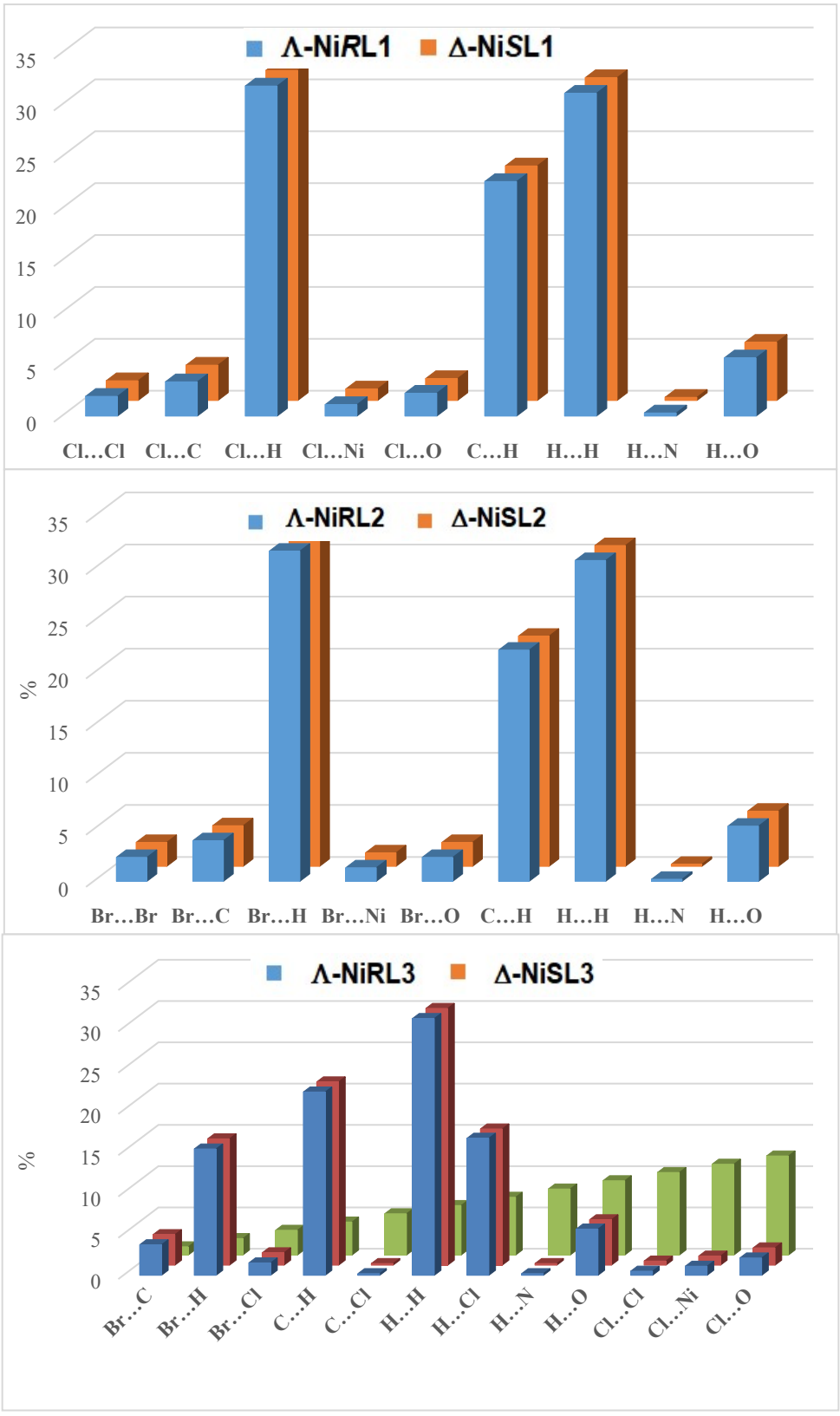


Fig. S3 Relative contributions to the Hirshfeld surfaces area for different intermolecular contacts in nickel(II)-Schiff bases complexes.

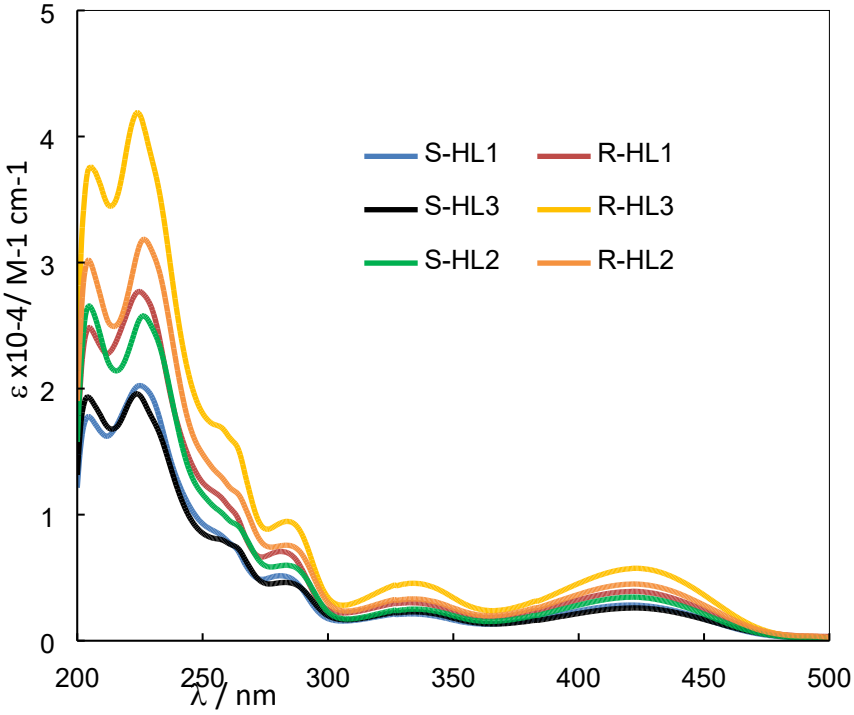


Fig. S4 UV-Vis. spectra for Schiff bases *R*-HL[1]/*S*-HL[1] (3.24/3.22x10^{-2} mM), *R*-HL[2]/*S*-HL[2] (2.45/3.09x10^{-2} mM) and *R*-HL[3]/*S*-HL[3] (2.79/3.10x10^{-2} mM) in methanol at 25 °C.

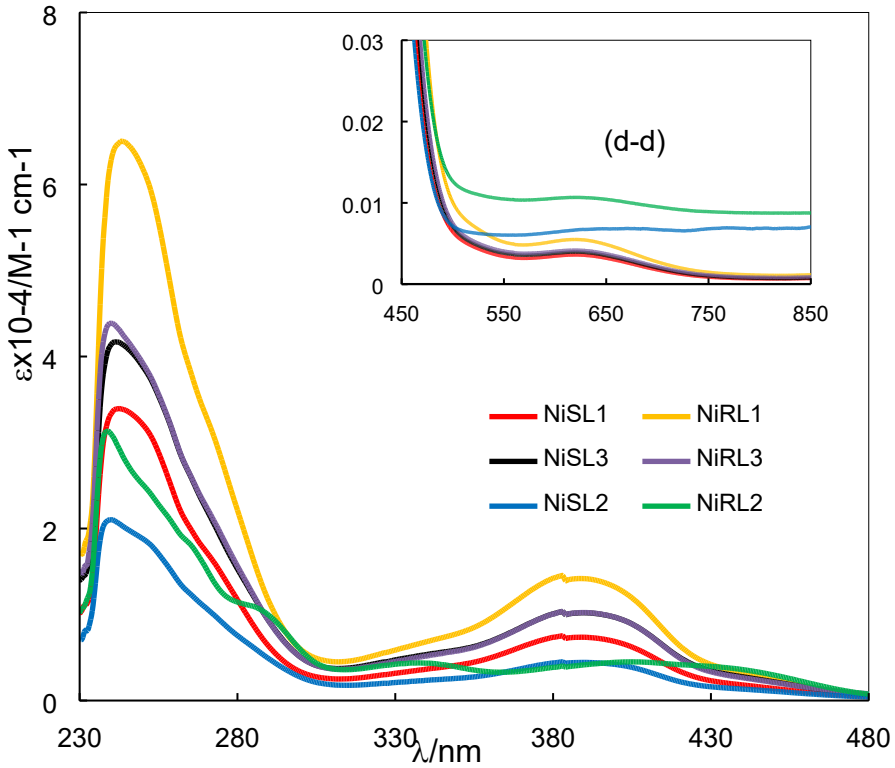
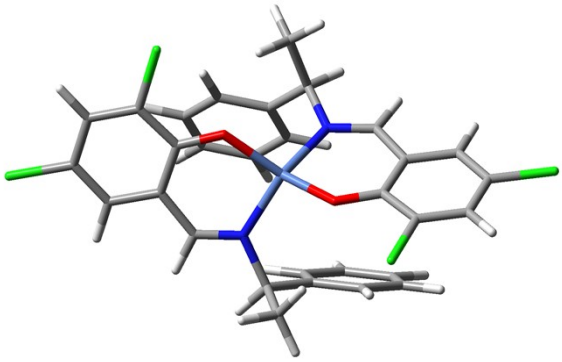
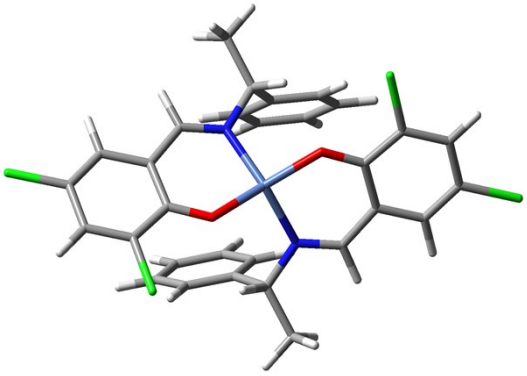
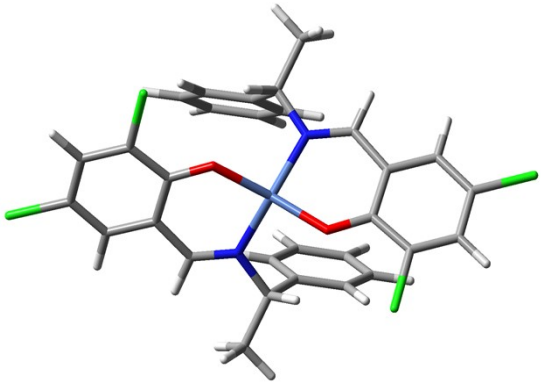
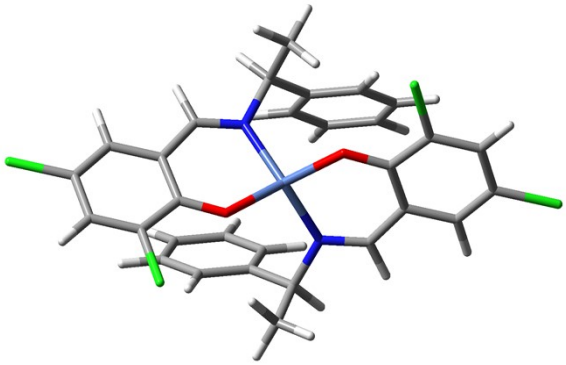
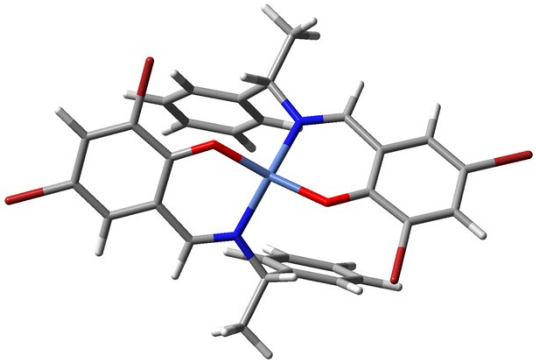
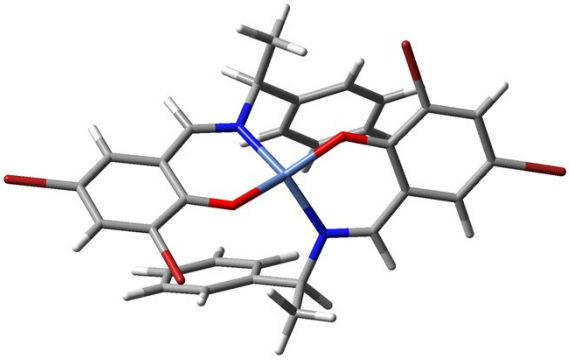
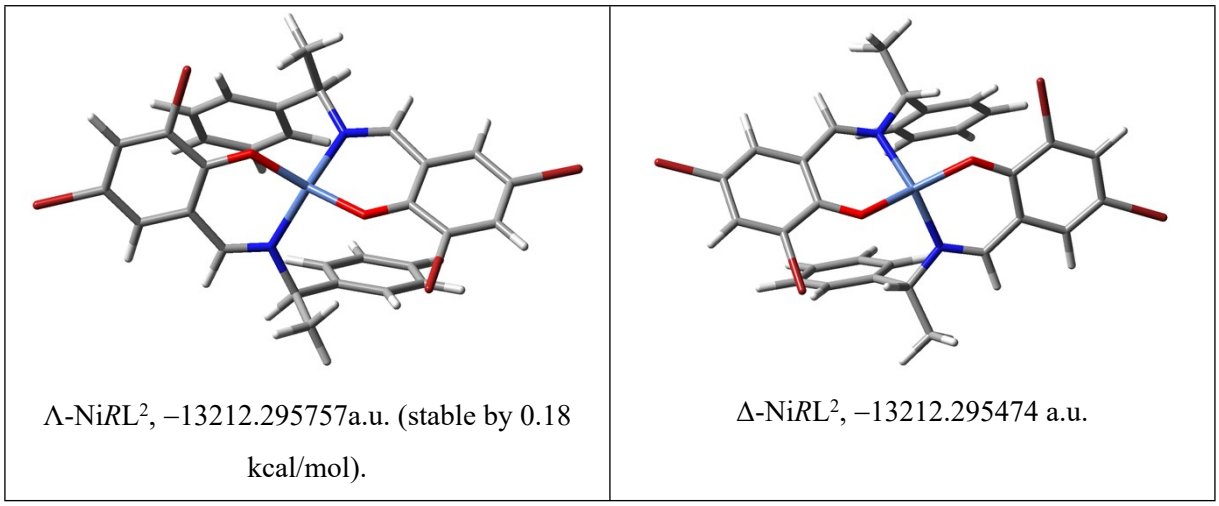


Fig. S5 UV-Vis. spectra for Ni*R*L[1]/Ni*S*L[1] (2.00/2.84x10^{-2} mM), Ni*R*L[2]/Ni*S*L[2] (1.76/2.29x10^{-2} mM) and Ni*R*L[3]/Ni*S*L[3] (1.44/1.89x10^{-2} mM) in methanol/chloroform (50%, v/v) at 25 °C.

Λ-diastereomer	Δ-diastereomer
 Λ-Zn*R*L[1], –4766.249579 a.u. (stable by 1.69 kcal/mol).	 Δ-Ni*R*L[1], –4766.246884 a.u.
 Λ-Ni*S*L[1], –4766.249428 a.u.	 Δ-Ni*S*L[1], –4766.249580 a.u. (stable by 0.10 kcal/mol).
 Λ-Ni*S*L[2], –13212.295473 a.u.	 Δ-Ni*S*L[2], –13212.295757 a.u. (stable by 0.18 kcal/mol).



Λ-Ni*R*L^2, −13212.295757a.u. (stable by 0.18 kcal/mol).

Δ-Ni*R*L^2, −13212.295474 a.u.

Fig. S6 DFT optimized structures for the diastereomeric pairs of Λ-Ni*R*L$^{1-2}$/Δ-Ni*R*L$^{1-2}$ and Δ-Ni*S*L$^{1-2}$/Λ-Ni*S*L$^{1-2}$ at b3lyp/6-31G(d), respectively.

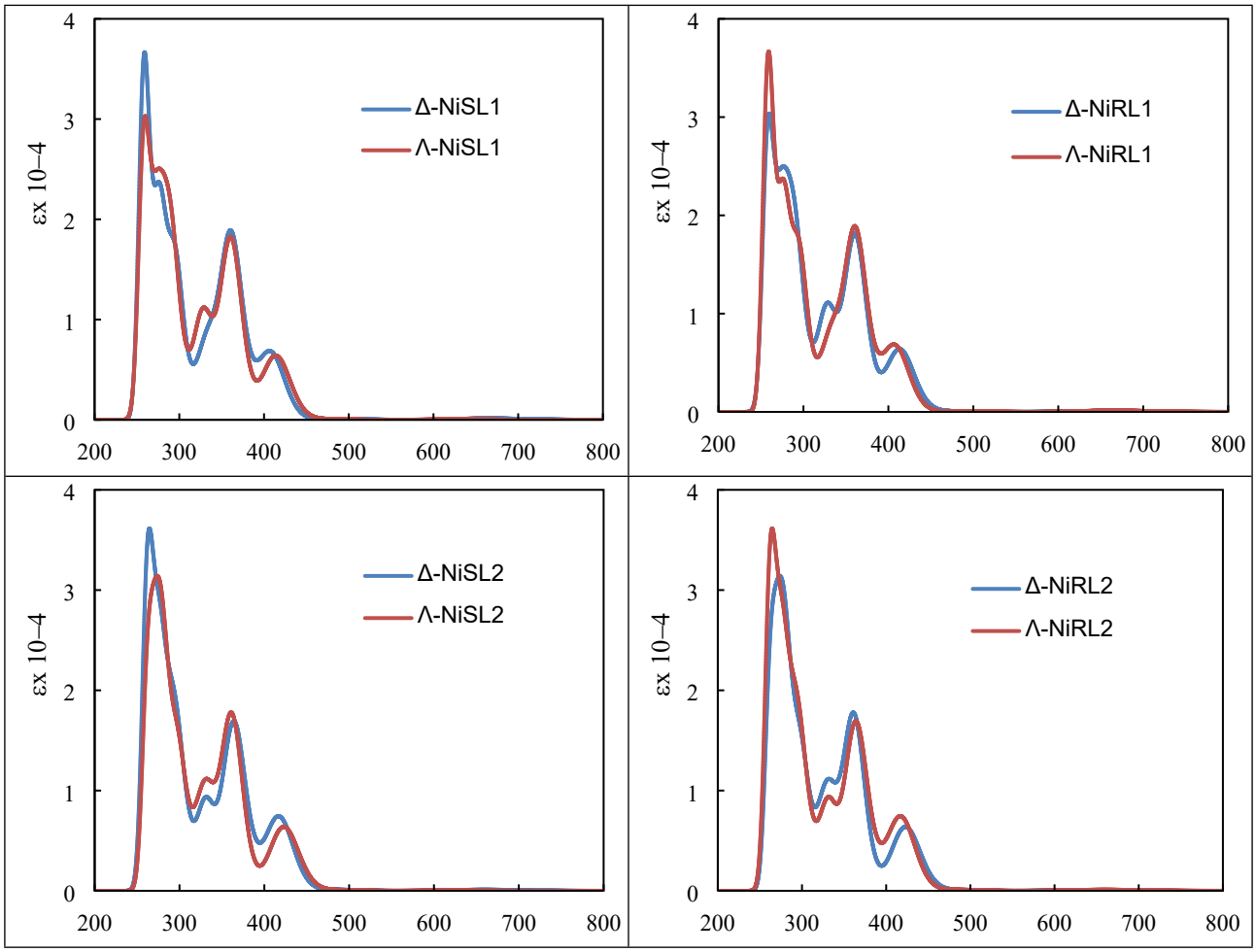


Fig. S7 Simulated UV-Vis. spectra for diastereomeric pairs of Λ-Ni*S*L$^{1-2}$/Δ-Ni*S*L$^{1-2}$ and Λ-Ni*R*L$^{1-2}$/Δ-Ni*R*L$^{1-2}$ at b3lyp/6-31G(d) with PCM in chloroform. Gaussian band shape with exponential half-width σ = 0.16 eV.

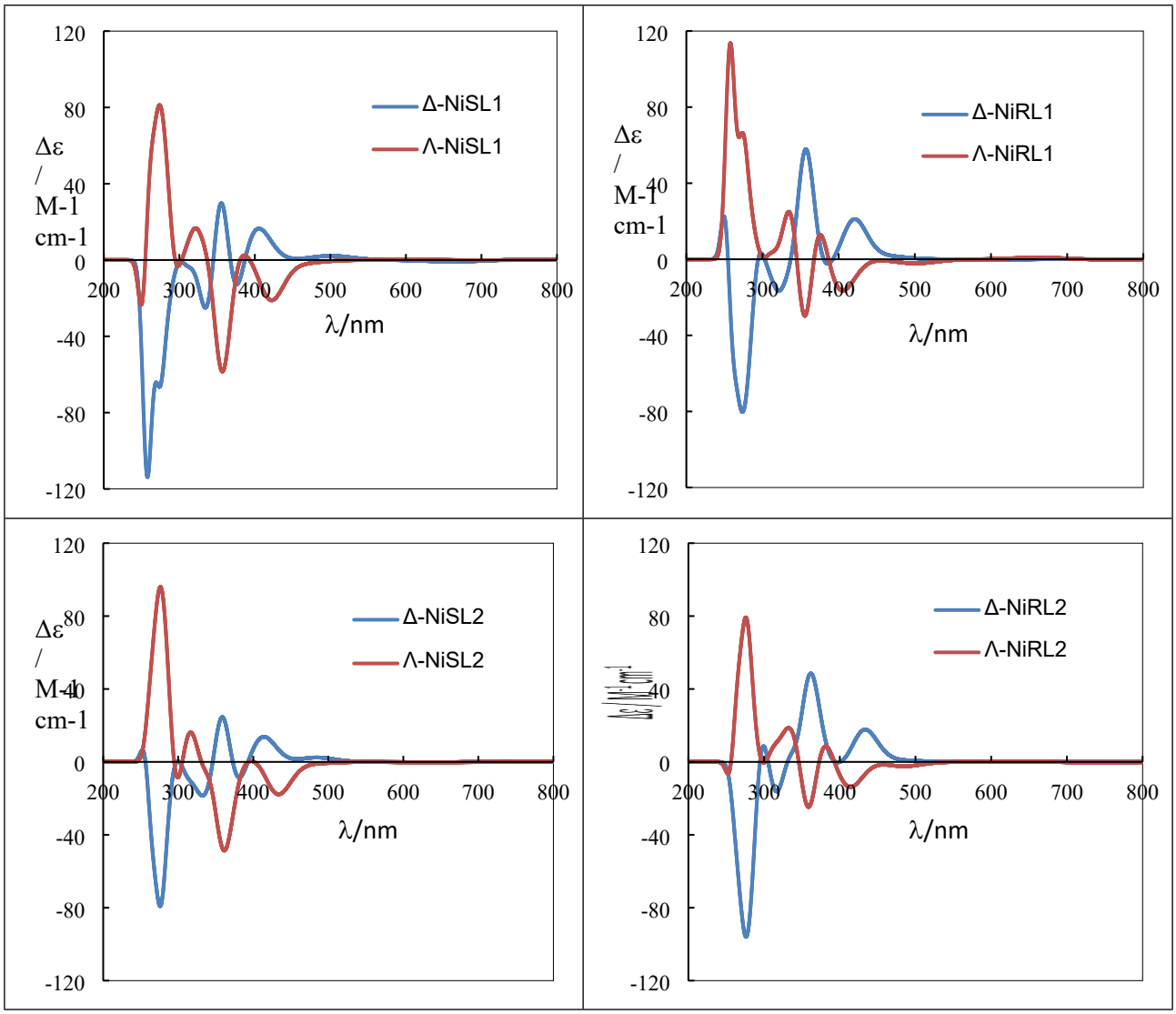
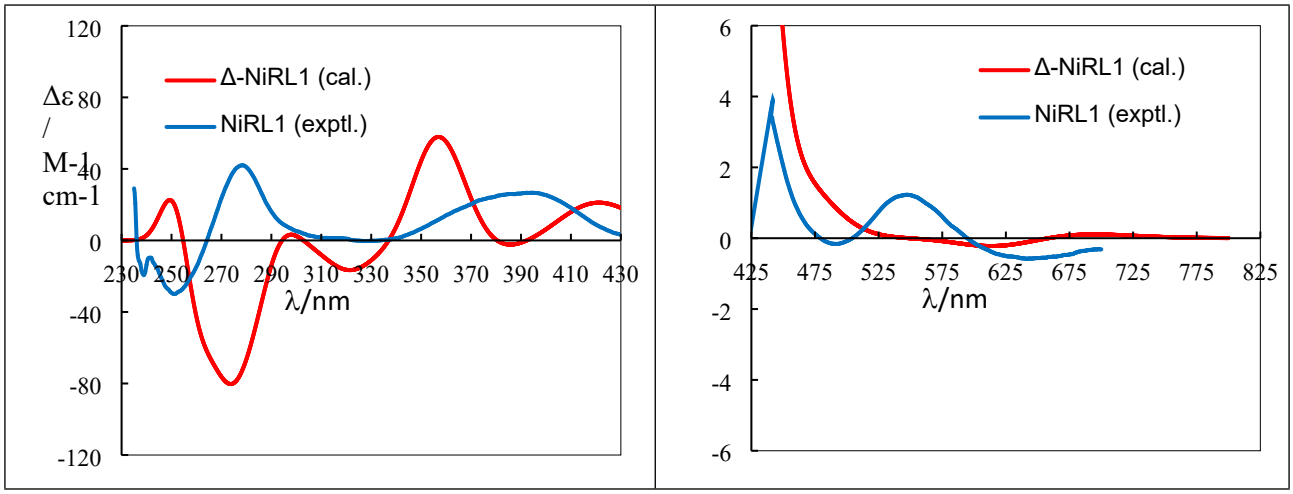


Fig. S8 Simulated ECD spectra for diastereomeric pairs Λ-Ni*S*L$^{1\text{-}2}$/Δ-Ni*S*L$^{1\text{-}2}$ and Λ-Ni*R*L$^{1\text{-}2}$/Δ-Ni*R*L$^{1\text{-}2}$ at b3lyp/6-31G(d) with PCM in chloroform. Gaussian band shape with exponential half-width σ = 0.16 eV.



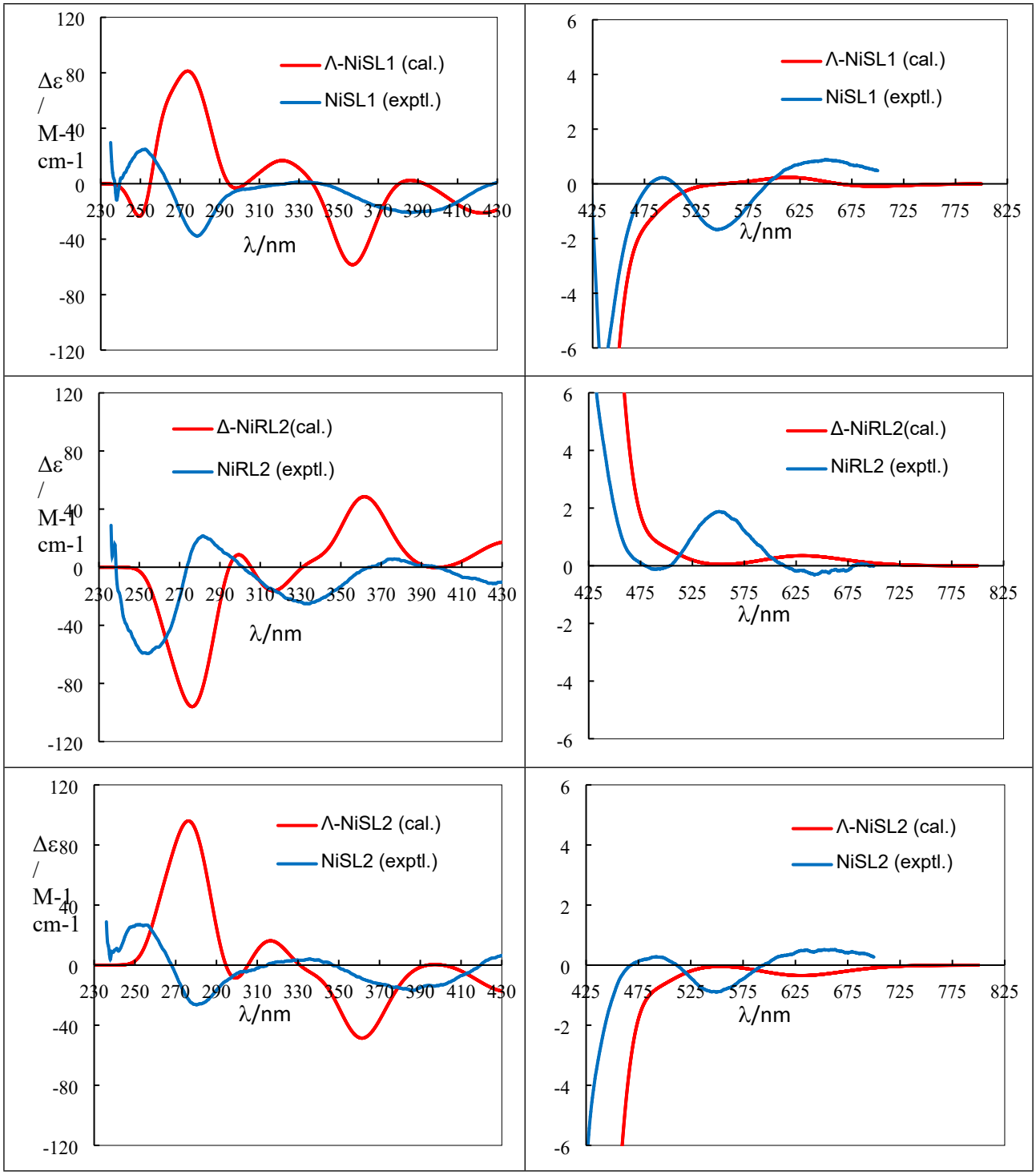
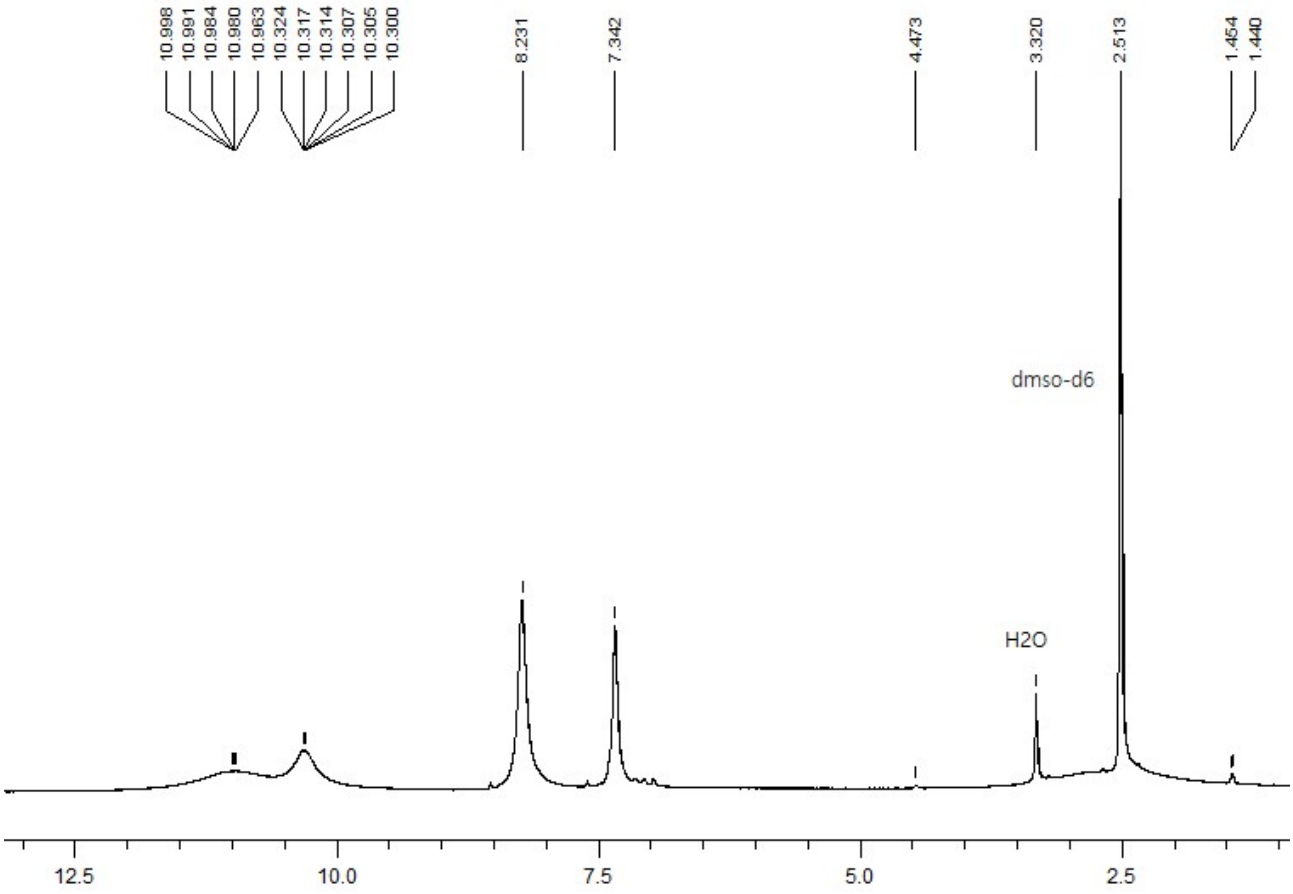


Fig. S9 Opposite matching of experimental and simulated ECD spectra: (a) experimental spectra (*ca.* 2.0x10^{-2} mM at 500-235 nm and *ca.* 1.0 mM at 700-425 nm) in methanol:chloroform (50%, v/v) at 20 °C ($\Delta\varepsilon_{exptl.}$ values are multiplied by 5); (b) simulated spectra calculated at b3lyp/6-31G(d) with PCM in chloroform. Gaussian band shape with exponential half-width σ = 0.16 eV.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10.991
10.984
10.980
10.963
10.324
10.317
10.314
10.307
10.305
10.300
8.231
7.342
4.473
3.320
2.513
1.454
1.440
dmso-d6
H2O
12.5
10.0
7.5
5.0
2.5

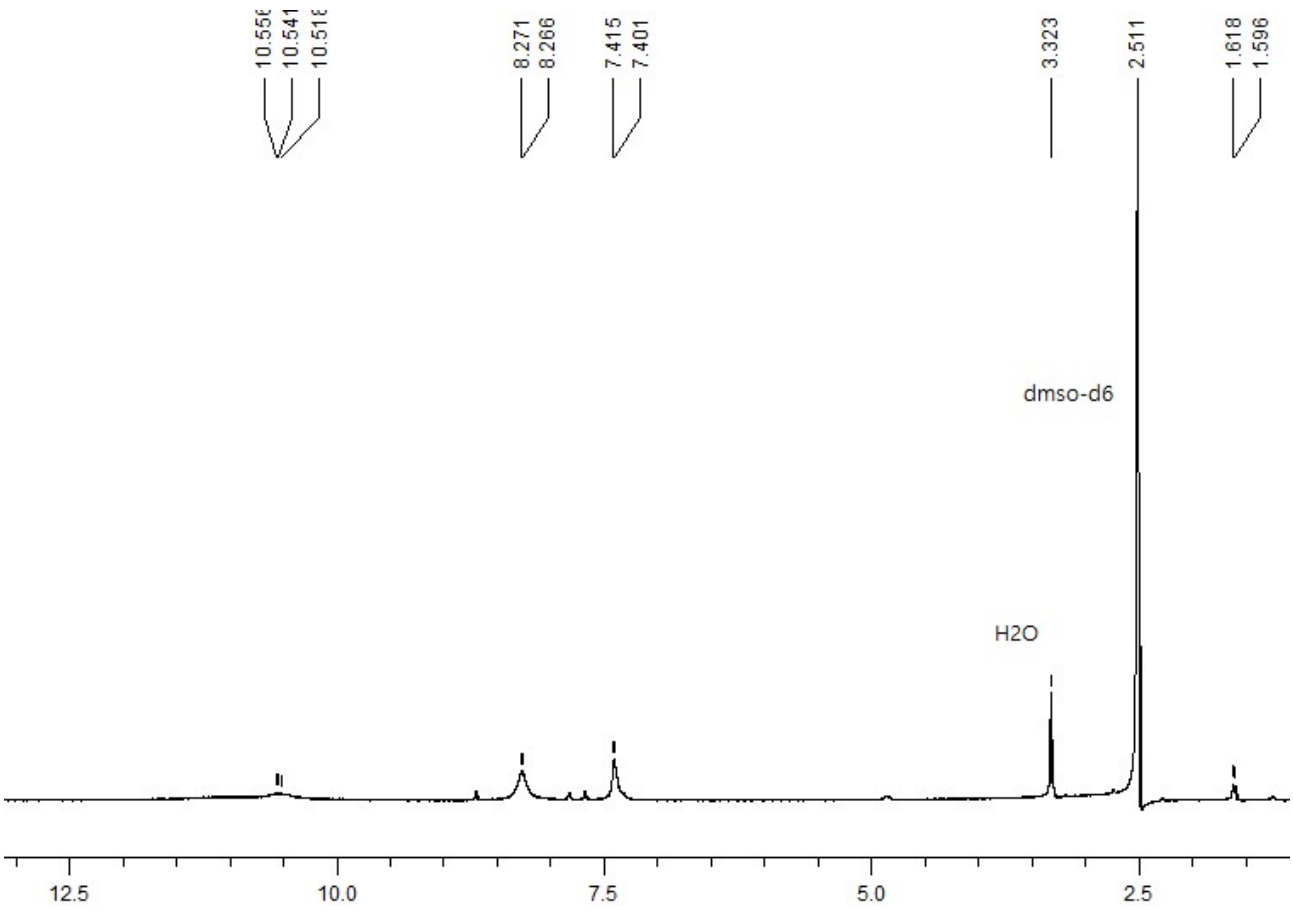
10.556
10.541
10.518
8.271
8.266
7.415
7.401
3.323
2.511
1.618
1.596
dmso-d6
H2O
12.5
10.0
7.5
5.0
2.5

Fig. S10 ^{1}H NNR spectrum for Ni*R*L^{1} (top) and Ni*R*L^{2} (bottom) in dmso-d_6 at 20 °C.

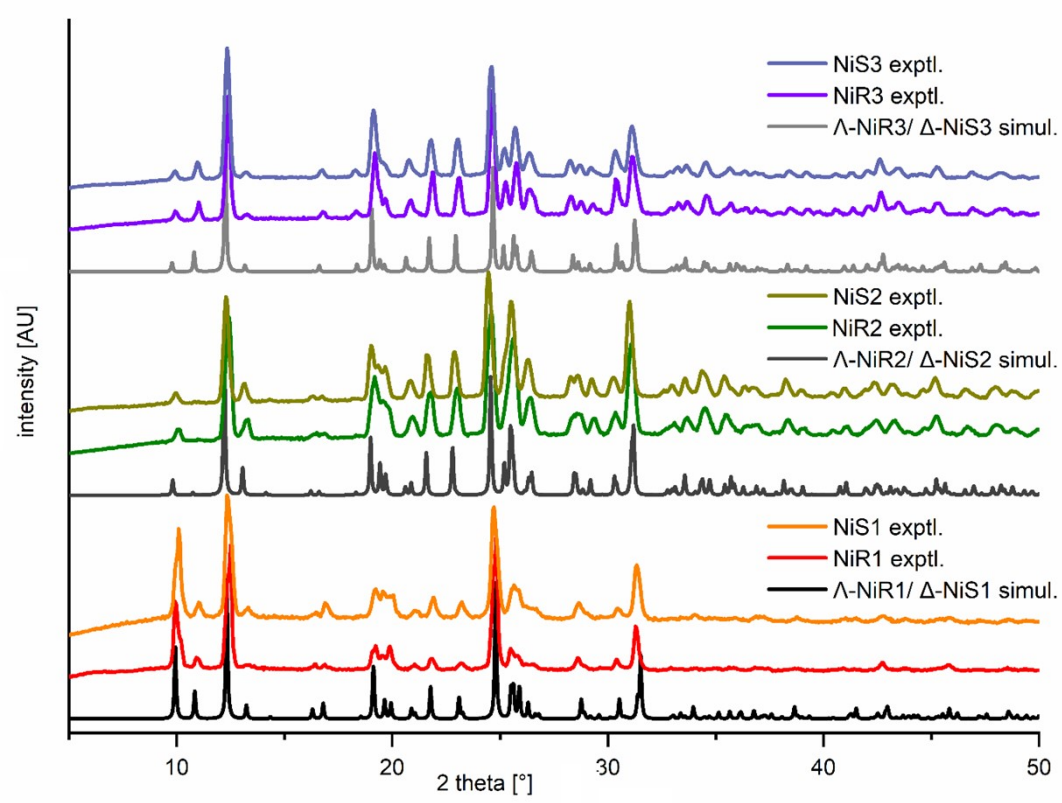

Fig. S11. Experimental and simulated PXRD patterns (from single crystal X-ray structure) for Ni*R*L$^{1-3}$ and Ni*S*L$^{1-3}$ at ambient temperature.

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

	Λ-Ni*R*L^{1}	Λ-Ni*R*L^{2}	Λ-Ni*R*L^{3}	Δ-Ni*S*L^{1}	Δ-Ni*S*L^{2}	Δ-Ni*S*L^{3}
Empirical formula	$C_{30}H_{24}Cl_4NiN_2O_2$	$C_{30}H_{24}Br_4NiN_2O_2$	$C_{30}H_{24}Br_2Cl_2NiN_2O_2$	$C_{30}H_{24}Cl_4NiN_2O_2$	$C_{30}H_{24}Br_4NiN_2O_2$	$C_{30}H_{24}Br_4NiN_2O_2$
M (g mol^{-1})	645.02	822.86	733.94	645.02	822.86	733.94
Temperature (K)	160(1)	160(1)	160(1)	160(1)	160(1)	160(1)
Wavelength (Å)	1.54184	0.71073	0.71073	0.71073	1.54184	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	I2	I2	I2	I2	I2	I2
a (Å)	9.98147(15)	10.1024(2)	10.1101(2)	9.9679(2)	10.10590(10)	10.09670(10)
b (Å)	10.86524(17)	10.91929(18)	10.85749(19)	10.8655(2)	10.93120(10)	10.85000(10)
c (Å)	12.8851(2)	13.0659(3)	13.0218(3)	12.8831(4)	13.06820(10)	13.0172(2)
β (°)	106.6972(17)	106.645(2)	107.285(2)	106.713(3)	106.6210(10)	107.3140(10)
V(Å$^{3)}$	1338.49(4)	1380.91(5)	1364.86(5)	1336.37(6)	1383.32(2)	1361.41(3)
Z	2	2	2	2	2	2
$D_{calc.}$(g cm^{-3})	1.600	1.979	1.786	1.603	1.976	1.790
μ (mm^{-1})	4.989	6.522	3.867	1.159	8.042	3.877
F(000)	660.0	804.0	732.0	660.0	804.0	732.0
θ range (°)	9.942 to 148.978	5.624 to 52.74	4.98 to 52.734	4.996 to 52.738	9.818 to 148.848	4.512 to 52.738

h; *k*; *l* ranges	-9,+12; ±13; ±16	±12; ±13; ±16	±12; ±13; ±16	±12; ±13; ±16	±12; ±13; ±16	±12; ±13; ±16
Reflections collected	13792	13776	14452	13534	14700	17509
Independent reflect. (R_{int})	2723 (0.0243)	2849 (0.0484)	2797 (0.0226)	2722 (0.0288)	2850 (0.0242)	2792 (0.0272)
Data/restraints/parameters	2723/1/178	2849/1/178	2797/1/178	2722/1/178	2850/1/178	2792/1/178
Goodness-of-fit on F^2 [a]	1.058	1.028	1.045	1.054	1.073	1.064
R_1/wR_2 [I>2σ (I)] [b]	0.0219/0.0571	0.0335/0.0841	0.0131/0.0334	0.0256/0.0647	0.0174/0.0461	0.0136/0.0325
R_1/wR_2 (all data) [b]	0.0225/0.0573	0.0352/0.0856	0.0134/0.0335	0.0272/0.0659	0.0174/0.0461	0.0141/0.0327
Max./min. $\Delta\rho$ (e. Å^{-3}) [c]	0.22/-0.20	1.46/-0.49	0.27/-0.15	0.52/-0.34	0.25/-0.44	0.18/-0.16
Flack parameter [d]	-0.006(6)	-0.004(9)	-0.005(3)	-0.024(5)	-0.019(9)	-0.006(3)
CCDC number	2000645	2000643	2000647	2000651	2000649	2149672

[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.[1,2]

Table S2. Excited state properties for Λ-Ni*R*L[1] (Excited states, excitation energy (eV), wavelength (nm) and oscillator strength (*f*)), calculated at b3lyp/6-31G(d) with PCM in chloroform.

Excitation energies and oscillator strengths:

Excited State 1: 3.002-A 0.6374 eV 1945.23 nm f=0.0000 <S**2>=2.002

154B ->165B	0.36478
154B ->167B	0.31260
155B ->165B	-0.18294
155B ->167B	-0.15585
157B ->165B	-0.22285
157B ->167B	-0.18537
158B ->168B	0.27506
159B ->165B	-0.30147
159B ->167B	-0.24991
160B ->168B	0.23529
162B ->165B	0.42360
162B ->167B	0.34440
163B ->165B	-0.12719
163B ->167B	-0.11074
164B ->168B	0.13841
154B <-165B	0.10513
158B <-168B	0.12141
160B <-168B	0.10318
162B <-165B	0.10826

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -4766.63597251

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.005-A 0.7600 eV 1631.33 nm f=0.0000 <S**2>=2.007

153B ->165B	-0.13833
153B ->167B	-0.11687
154B ->168B	-0.14650
158B ->165B	0.50863
158B ->167B	0.41533
160B ->165B	0.43744
160B ->167B	0.35777
164B ->165B	0.27444
164B ->167B	0.21558

Excited State 3: 3.004-A 1.0571 eV 1172.89 nm f=0.0014 <S**2>=2.006

138B ->165B	0.10563
148B ->165B	0.18155
148B ->167B	0.15788
150B ->165B	-0.11483
150B ->167B	-0.10073
153B ->168B	0.11842
154B ->165B	0.42210
154B ->167B	0.35222
155B ->165B	0.29587
155B ->167B	0.24168
158B ->168B	-0.41628
160B ->168B	-0.35749
164B ->168B	-0.20632

Excited State 4: 3.003-A 1.6168 eV 766.84 nm f=0.0000 <S**2>=2.004

144B ->168B	0.11771
148B ->168B	0.25987
150B ->168B	-0.19562
155B ->168B	0.57792
157B ->168B	0.30083
159B ->168B	0.33894
162B ->168B	-0.43003
163B ->168B	0.28171

Excited State 5: 3.008-A 1.8630 eV 665.51 nm f=0.0014 <S**2>=2.012

148B ->165B	0.16901
148B ->167B	0.14272
150B ->165B	-0.11868
150B ->167B	-0.10090
153B ->168B	-0.12243

154B ->165B 0.19422
154B ->167B 0.15030
155B ->165B 0.37254
155B ->167B 0.29302
157B ->165B 0.13300
157B ->167B 0.10438
158B ->168B 0.44161
159B ->165B 0.12657
160B ->168B 0.38252
162B ->165B -0.14240
162B ->167B -0.10960
163B ->165B 0.20492
163B ->167B 0.14756
164B ->168B 0.25932

Excited State 6: 3.069-A 2.4337 eV 509.45 nm f=0.0004 <S**2>=2.105
165A ->168A -0.13183
166A ->167A -0.18102
138B ->168B 0.13384
148B ->168B 0.19229
150B ->168B -0.11207
151B ->168B -0.11526
154B ->168B 0.69471
155B ->168B 0.25221
157B ->168B -0.10909
159B ->168B -0.22323
162B ->168B 0.37238
164B ->165B 0.15996

Excited State 7: 4.012-A 2.5560 eV 485.08 nm f=0.0003 <S**2>=3.773
165A ->167A 0.49652
166A ->168A 0.52413
163B ->165B -0.43500
163B ->167B 0.22761
164B ->166B -0.44036

Excited State 8: 3.962-A 2.5642 eV 483.52 nm f=0.0001 <S**2>=3.674
165A ->168A 0.47230
166A ->167A 0.49904
154B ->168B 0.18763
163B ->166B -0.40859
164B ->165B -0.42617

164B ->167B 0.26040

Excited State 9: 3.366-A 3.0280 eV 409.45 nm f=0.0503 <S**2>=2.582
158A ->168A -0.11448
159A ->167A -0.16408
164A ->168A -0.15676
165A ->167A 0.11992
166A ->168A 0.25127
155B ->165B -0.16927
156B ->166B 0.18141
162B ->167B 0.24652
163B ->165B 0.71853
163B ->167B 0.28488

Excited State 10: 3.439-A 3.0312 eV 409.02 nm f=0.0101 <S**2>=2.707
158A ->167A -0.11653
159A ->168A -0.16801
164A ->167A -0.18211
165A ->168A 0.12146
166A ->167A 0.29056
156B ->165B 0.11913
156B ->167B -0.15348
158B ->167B -0.18555
160B ->165B -0.17715
162B ->166B -0.26690
164B ->165B 0.67997
164B ->167B 0.23899

Excited State 11: 3.832-A 3.1593 eV 392.44 nm f=0.0088 <S**2>=3.421
157A ->167A 0.10931
158A ->168A 0.18015
159A ->167A 0.26257
160A ->168A 0.12418
161A ->168A 0.10184
162A ->167A 0.12783
164A ->168A 0.32371
165A ->167A 0.25711
165A ->173A 0.10946
166A ->170A 0.11460
166A ->174A -0.10019
154B ->165B -0.10924
155B ->167B -0.12124

156B ->166B -0.25431
158B ->166B -0.10756
162B ->165B 0.33763
162B ->167B -0.15439
163B ->165B 0.34100
163B ->167B 0.26537
163B ->170B -0.11021
163B ->174B 0.10514
164B ->166B -0.23948
164B ->168B 0.11851
164B ->173B -0.11633

Excited State 12: 3.739-A 3.1636 eV 391.91 nm f=0.0010 <S**2>=3.246
158A ->167A 0.18080
159A ->168A 0.25923
160A ->167A 0.12565
162A ->168A 0.12229
164A ->167A 0.32151
165A ->168A 0.25274
165A ->170A 0.10276
166A ->173A 0.10663
156B ->165B -0.23308
156B ->167B 0.14252
158B ->165B -0.19523
160B ->167B -0.13040
162B ->166B 0.29281
163B ->166B -0.26338
163B ->168B 0.15667
163B ->173B -0.10945
164B ->165B 0.40882
164B ->167B 0.21567
164B ->170B -0.11069
164B ->174B 0.10600

Excited State 13: 3.442-A 3.2650 eV 379.73 nm f=0.0050 <S**2>=2.711
158A ->167A 0.13178
159A ->168A 0.19858
161A ->167A 0.13179
164A ->167A -0.20978
165A ->168A -0.45872
166A ->167A 0.72161
162B ->166B 0.13107

163B ->166B 0.14578
164B ->167B -0.13800

Excited State 14: 3.471-A 3.2793 eV 378.08 nm f=0.0073 <S**2>=2.762
158A ->168A 0.13667
159A ->167A 0.20888
161A ->168A 0.13176
164A ->168A -0.19034
165A ->167A -0.46043
166A ->168A 0.72666
156B ->166B -0.12364
162B ->165B 0.11301
164B ->166B 0.12142

Excited State 15: 3.076-A 3.4157 eV 362.98 nm f=0.1015 <S**2>=2.115
165A ->167A 0.57630
166A ->168A 0.16844
163B ->167B -0.12921
164B ->166B 0.74797
164B ->168B 0.11655

Excited State 16: 3.226-A 3.4473 eV 359.66 nm f=0.0638 <S**2>=2.352
165A ->168A 0.63088
166A ->167A 0.14554
163B ->166B 0.61646
164B ->167B -0.38721

Excited State 17: 3.517-A 3.5375 eV 350.48 nm f=0.0003 <S**2>=2.843
158B ->165B -0.14598
160B ->165B -0.12463
163B ->166B 0.56498
164B ->165B -0.23849
164B ->167B 0.73939

Excited State 18: 3.657-A 3.5479 eV 349.46 nm f=0.0215 <S**2>=3.093
164A ->168A 0.10328
165A ->167A -0.24808
163B ->165B -0.27515
163B ->167B 0.80085
164B ->166B 0.35824
164B ->168B -0.12483

Excited State 19: 3.221-A 3.6893 eV 336.07 nm f=0.0578 <S**2>=2.344

159A ->167A	-0.10994
164A ->168A	-0.17059
166A ->168A	-0.10741
158B ->168B	-0.22632
160B ->168B	-0.19615
163B ->167B	0.15527
164B ->168B	0.83565

Excited State 20: 3.547-A 3.7145 eV 333.79 nm f=0.0014 <S**2>=2.895

161A ->169A	-0.14740
162A ->170A	0.11699
163A ->172A	0.16176
164A ->167A	-0.32646
165A ->174A	-0.10854
166A ->167A	-0.11268
155B ->168B	-0.10277
157B ->171B	-0.11121
159B ->169B	-0.13562
160B ->170B	0.10192
161B ->172B	-0.15886
162B ->168B	0.12426
163B ->168B	0.68953
164B ->174B	0.10742

Excited State 21: 4.107-A 3.7220 eV 333.11 nm f=0.0018 <S**2>=3.966

158A ->172A	-0.17805
160A ->170A	-0.16147
160A ->172A	0.13236
160A ->174A	-0.16871
161A ->170A	0.18189
161A ->172A	0.21591
162A ->169A	-0.21046
162A ->171A	0.17013
162A ->173A	0.17063
163A ->169A	-0.30489
163A ->171A	-0.19942
163A ->173A	-0.11139
156B ->169B	-0.11101
157B ->172B	0.23438
157B ->174B	-0.12336
158B ->169B	0.12446

158B ->171B -0.12560
159B ->170B 0.22798
159B ->172B 0.11941
159B ->174B 0.14471
160B ->169B -0.12181
160B ->171B 0.19330
160B ->173B 0.10217
161B ->169B 0.32160
161B ->171B 0.19082
162B ->172B 0.14601
164B ->168B -0.11951

Excited State 22: 3.961-A 3.7311 eV 332.30 nm f=0.0006 <S**2>=3.672
158A ->169A -0.12105
158A ->171A -0.10388
160A ->171A 0.18378
160A ->173A 0.15459
161A ->169A 0.28924
162A ->170A -0.21392
162A ->174A -0.18007
163A ->172A -0.31167
164A ->167A -0.16454
157B ->171B 0.21723
158B ->170B 0.13278
159B ->169B 0.25085
159B ->171B -0.10673
160B ->170B -0.16415
160B ->174B -0.14373
161B ->172B 0.31017
162B ->169B 0.16092
163B ->168B 0.37257

Excited State 23: 3.439-A 3.8309 eV 323.65 nm f=0.0033 <S**2>=2.707
157A ->168A 0.14639
158A ->167A -0.16632
159A ->168A -0.21501
160A ->167A -0.12929
161A ->167A -0.25267
164A ->167A 0.70491
165A ->168A -0.19711
166A ->167A 0.23963
155B ->166B -0.10358

163B ->166B 0.10698
163B ->168B 0.35198

Excited State 24: 3.449-A 3.8333 eV 323.44 nm f=0.0258 <S**2>=2.723
157A ->167A 0.17323
158A ->168A -0.12082
159A ->167A -0.15971
161A ->168A -0.22486
164A ->168A 0.77855
165A ->167A -0.19696
166A ->168A 0.24828
163B ->167B -0.15613
164B ->168B 0.18398

Excited State 25: 3.811-A 3.9056 eV 317.46 nm f=0.0002 <S**2>=3.381
164A ->167A -0.14887
165A ->170A -0.27867
165A ->174A 0.24370
166A ->171A 0.26379
166A ->173A -0.25979
157B ->166B -0.11097
158B ->165B -0.14199
159B ->166B -0.15996
161B ->165B -0.19845
162B ->166B 0.37916
162B ->168B 0.10920
163B ->168B 0.26163
163B ->171B -0.17367
163B ->173B 0.29812
164B ->170B 0.24424
164B ->174B -0.23519

Excited State 26: 3.828-A 3.9109 eV 317.03 nm f=0.0006 <S**2>=3.414
161A ->168A 0.11486
164A ->168A -0.17930
165A ->171A 0.25867
165A ->173A -0.26400
166A ->170A -0.27715
166A ->174A 0.24452
158B ->166B -0.27532
159B ->167B 0.11041
160B ->166B -0.17688

162B ->165B 0.31690
162B ->167B -0.23498
163B ->170B 0.23796
163B ->174B -0.23052
164B ->168B 0.19071
164B ->171B -0.17140
164B ->173B 0.30087

Excited State 27: 3.301-A 3.9929 eV 310.51 nm f=0.0012 <S**2>=2.474
158B ->165B 0.16223
161B ->165B 0.93084
161B ->167B 0.10321
162B ->166B 0.11084

Excited State 28: 3.704-A 4.0003 eV 309.94 nm f=0.0113 <S**2>=3.180
165A ->171A 0.11555
165A ->173A -0.11011
166A ->170A -0.12179
166A ->174A 0.11447
155B ->165B 0.10750
158B ->166B 0.58639
160B ->166B 0.65397
161B ->166B -0.15085
163B ->167B -0.10007
164B ->166B -0.14102
164B ->173B 0.10304

Excited State 29: 3.579-A 4.0499 eV 306.14 nm f=0.0014 <S**2>=2.953
153B ->165B 0.17229
155B ->166B 0.11752
158B ->165B 0.17549
158B ->167B -0.47291
160B ->165B 0.65663
160B ->167B -0.42566

Excited State 30: 3.225-A 4.0747 eV 304.28 nm f=0.0180 <S**2>=2.350
159A ->167A -0.13203
158B ->166B 0.10544
159B ->165B 0.69860
159B ->167B 0.11387
162B ->165B 0.59372
162B ->167B 0.14832

Excited State 31: 3.301-A 4.0982 eV 302.53 nm f=0.0002 <S**2>=2.474

158B ->165B	0.72567
160B ->165B	-0.52370
160B ->167B	-0.27796
161B ->165B	-0.20405
162B ->166B	0.11316

Excited State 32: 3.607-A 4.1860 eV 296.19 nm f=0.0020 <S**2>=3.003

159A ->168A	-0.13867
164A ->167A	-0.12729
165A ->170A	0.10296
153B ->165B	-0.22394
154B ->166B	0.18865
155B ->166B	-0.32475
156B ->165B	0.41092
157B ->166B	-0.17761
158B ->167B	-0.14821
159B ->166B	-0.27814
162B ->166B	0.48900
163B ->168B	-0.12661
163B ->173B	-0.13264
164B ->167B	0.14593
164B ->170B	-0.12187
164B ->174B	0.12599

Excited State 33: 3.599-A 4.1903 eV 295.89 nm f=0.1064 <S**2>=2.987

158A ->168A	0.10713
159A ->167A	0.23747
160A ->168A	0.10565
161A ->168A	0.11700
163A ->167A	-0.24148
164A ->168A	0.14184
154B ->167B	0.16859
155B ->165B	0.17611
155B ->167B	-0.25981
156B ->166B	-0.17314
157B ->167B	-0.18378
158B ->166B	-0.14539
159B ->165B	0.47073
159B ->167B	-0.23240
162B ->165B	-0.28648

162B ->167B 0.36486

Excited State 34: 3.899-A 4.2360 eV 292.69 nm f=0.0145 <S**2>=3.551
162A ->167A 0.13528
163A ->167A 0.82421
164A ->168A -0.10416
157B ->165B -0.17386
159B ->165B 0.20315
161B ->166B -0.35107
162B ->165B -0.18720

Excited State 35: 3.626-A 4.2520 eV 291.59 nm f=0.0047 <S**2>=3.037
159A ->168A -0.10809
162A ->168A 0.15609
163A ->168A 0.94924
164A ->167A -0.12725

Excited State 36: 3.230-A 4.2690 eV 290.43 nm f=0.0064 <S**2>=2.359
163A ->167A 0.38609
154B ->165B -0.15875
155B ->165B 0.22044
157B ->165B 0.58592
159B ->165B -0.17830
161B ->166B 0.49828
162B ->165B 0.13603
162B ->167B 0.22377

Excited State 37: 3.290-A 4.3066 eV 287.89 nm f=0.0003 <S**2>=2.456
157A ->168A -0.11119
159A ->168A 0.16380
161A ->167A 0.33606
164A ->167A 0.17069
153B ->165B 0.23965
155B ->166B 0.15337
156B ->165B 0.74262
156B ->167B 0.20326
158B ->167B 0.20747
159B ->166B 0.12855
161B ->167B 0.14052

Excited State 38: 3.364-A 4.3124 eV 287.50 nm f=0.0098 <S**2>=2.579
162A ->167A 0.20245

163A ->167A 0.11565
155B ->165B -0.11360
157B ->165B -0.51146
158B ->166B 0.11371
159B ->165B 0.16600
161B ->166B 0.71226
162B ->165B -0.11268
162B ->167B -0.19712

Excited State 39: 3.669-A 4.3376 eV 285.84 nm f=0.0054 <S**2>=3.115
157A ->167A 0.18748
159A ->167A -0.24682
160A ->168A 0.15543
161A ->168A -0.32171
162A ->167A 0.77433
163A ->167A -0.21651
164A ->168A -0.17800
161B ->166B -0.20566

Excited State 40: 3.667-A 4.3486 eV 285.11 nm f=0.0000 <S**2>=3.112
157A ->168A 0.16252
159A ->168A -0.15089
160A ->167A 0.21583
161A ->167A -0.32810
162A ->168A 0.80591
163A ->168A -0.15623
164A ->167A -0.13347
156B ->165B 0.20756
156B ->167B 0.10772

Excited State 41: 3.790-A 4.3899 eV 282.43 nm f=0.0227 <S**2>=3.341
157A ->167A -0.10737
158A ->168A -0.13136
159A ->167A -0.10093
160A ->168A -0.11721
161A ->168A 0.57423
162A ->167A 0.26125
154B ->165B 0.19989
155B ->165B -0.35602
156B ->166B 0.16886
157B ->165B 0.30945
158B ->166B -0.23033

160B ->166B 0.25542
161B ->166B 0.11267

Excited State 42: 3.888-A 4.3955 eV 282.07 nm f=0.0007 <S**2>=3.529
158A ->167A -0.20587
159A ->168A -0.26226
160A ->167A -0.17833
161A ->167A 0.58160
162A ->168A 0.35182
163A ->168A -0.13697
163A ->172A 0.11327
153B ->165B -0.13282
155B ->166B -0.11292
156B ->165B -0.16162
156B ->167B -0.15757
159B ->166B 0.40600
161B ->172B -0.11754
162B ->166B 0.13792

Excited State 43: 3.317-A 4.4088 eV 281.22 nm f=0.0281 <S**2>=2.500
157A ->167A 0.10754
158A ->168A 0.10913
161A ->168A -0.41022
162A ->167A -0.32340
154B ->167B 0.11758
155B ->165B -0.22558
158B ->166B -0.51947
160B ->166B 0.54788

Excited State 44: 3.130-A 4.4101 eV 281.13 nm f=0.0139 <S**2>=2.200
161A ->167A -0.48124
162A ->168A -0.15283
157B ->166B 0.10343
159B ->166B 0.71906
161B ->167B 0.12028
162B ->166B 0.39009

Excited State 45: 3.306-A 4.4346 eV 279.58 nm f=0.0285 <S**2>=2.482
159A ->167A -0.21236
160A ->168A -0.22735
161A ->168A 0.32539
154B ->165B -0.22215

154B ->167B -0.15883
155B ->165B 0.48691
156B ->166B 0.12139
157B ->165B -0.38443
158B ->166B -0.27517
159B ->165B -0.14792
159B ->167B 0.12029
160B ->166B 0.25638
162B ->165B 0.10352
162B ->167B 0.24579

Excited State 46: 3.378-A 4.4514 eV 278.53 nm f=0.0020 <S**2>=2.603
155B ->166B -0.15914
157B ->166B -0.12789
158B ->167B 0.12106
161B ->167B 0.92021
162B ->166B -0.14197

Excited State 47: 3.532-A 4.4877 eV 276.27 nm f=0.0049 <S**2>=2.869
155A ->168A 0.11395
157A ->167A 0.52251
159A ->167A -0.25714
160A ->168A 0.12961
161A ->168A 0.34517
162A ->167A -0.16911
148B ->165B 0.12308
150B ->165B -0.10551
154B ->165B -0.22993
154B ->167B 0.25879
155B ->165B -0.25237
155B ->167B 0.11870
156B ->166B -0.26860
158B ->166B 0.14270
159B ->167B 0.14924
162B ->167B 0.11162

Excited State 48: 3.573-A 4.5019 eV 275.40 nm f=0.0006 <S**2>=2.941
155A ->167A 0.14651
157A ->168A 0.52518
158A ->167A 0.11335
159A ->168A -0.16457
161A ->167A 0.14588

162A ->168A -0.23011
152B ->165B -0.11339
153B ->165B -0.15658
154B ->166B -0.38808
155B ->166B -0.22812
156B ->167B 0.19196
158B ->167B 0.17939
159B ->166B 0.17123
160B ->167B -0.33591

Excited State 49: 3.847-A 4.5196 eV 274.32 nm f=0.0002 <S**2>=3.449
157A ->168A 0.30414
158A ->167A -0.15980
159A ->168A -0.37733
160A ->167A 0.54151
161A ->167A 0.19206
162A ->168A -0.15499
154B ->166B 0.16062
155B ->166B 0.25510
157B ->166B 0.29784
158B ->167B -0.11444
160B ->167B 0.16874
162B ->166B 0.14516

Excited State 50: 3.437-A 4.5227 eV 274.14 nm f=0.1198 <S**2>=2.702
157A ->167A -0.39484
159A ->167A 0.33171
162A ->167A 0.19456
148B ->165B 0.11411
150B ->165B -0.10689
154B ->165B -0.24930
154B ->167B 0.11758
155B ->165B -0.21442
155B ->167B 0.23470
157B ->167B 0.12188
159B ->165B -0.11843
159B ->167B 0.42097
162B ->167B 0.45365

Excited State 51: 3.392-A 4.5341 eV 273.45 nm f=0.0040 <S**2>=2.627
157A ->168A -0.19147
158A ->167A -0.11181

159A ->168A 0.14713
160A ->167A 0.51183
153B ->167B 0.12271
154B ->166B -0.32869
155B ->166B -0.49886
157B ->166B -0.21599
158B ->167B -0.22792
159B ->166B 0.21294
160B ->167B 0.20172
161B ->167B -0.14024

Excited State 52: 3.717-A 4.5455 eV 272.76 nm f=0.0053 <S**2>=3.204
158A ->168A -0.23628
159A ->167A -0.15818
160A ->168A 0.79497
163A ->169A 0.13770
154B ->165B 0.13271
154B ->167B -0.11795
156B ->166B 0.15574
159B ->167B 0.19419
161B ->169B -0.13211

Excited State 53: 3.599-A 4.5687 eV 271.38 nm f=0.0003 <S**2>=2.988
157A ->168A 0.29060
158A ->167A 0.21417
160A ->167A -0.30554
153B ->165B 0.15412
155B ->166B 0.13085
156B ->167B 0.21744
157B ->166B -0.30873
158B ->167B -0.45190
160B ->167B 0.55046
161B ->167B 0.11385

Excited State 54: 3.406-A 4.5999 eV 269.54 nm f=0.0015 <S**2>=2.650
157A ->167A 0.16426
158A ->168A 0.15428
160A ->168A -0.24461
153B ->166B 0.11951
154B ->165B 0.41585
154B ->167B -0.12744
155B ->167B -0.36904

157B ->165B 0.10450
159B ->167B 0.63685
162B ->167B 0.12016

Excited State 55: 3.455-A 4.6061 eV 269.18 nm f=0.0015 <S**2>=2.735
159A ->168A 0.16697
160A ->167A -0.34173
162A ->168A 0.15294
166A ->169A -0.13693
154B ->166B -0.25354
155B ->166B -0.22745
157B ->166B 0.66262
158B ->167B -0.13890
159B ->166B -0.13422
160B ->167B 0.14994
161B ->170B 0.10817
162B ->166B 0.16007

Excited State 56: 3.217-A 4.6138 eV 268.73 nm f=0.0044 <S**2>=2.338
154A ->167A -0.12798
158A ->167A 0.15183
159A ->168A -0.21683
148B ->168B 0.13553
150B ->168B -0.12384
152B ->165B 0.11575
153B ->165B 0.69280
153B ->167B 0.28868
155B ->166B -0.23165
156B ->165B -0.12082
156B ->167B -0.18860
158B ->167B 0.22702
162B ->166B 0.13933
163B ->168B -0.13423

Excited State 57: 3.960-A 4.6861 eV 264.58 nm f=0.0009 <S**2>=3.670
158A ->170A 0.10671
159A ->167A 0.13905
160A ->168A -0.13232
160A ->172A 0.22945
161A ->170A -0.15660
161A ->172A -0.11614
161A ->174A -0.10854

162A ->169A 0.29263
162A ->171A 0.12809
163A ->169A 0.10451
163A ->171A -0.23034
163A ->173A -0.18265
166A ->170A 0.11020
156B ->169B 0.10480
157B ->167B -0.25044
157B ->170B -0.10545
157B ->172B 0.19387
157B ->174B -0.11536
158B ->169B -0.16480
159B ->167B 0.22255
159B ->170B -0.13644
159B ->172B -0.18365
160B ->169B 0.22594
160B ->171B 0.13117
161B ->169B -0.11369
161B ->171B 0.26719
161B ->173B 0.11204
164B ->169B 0.11681

Excited State 58: 4.051-A 4.6934 eV 264.17 nm f=0.0004 <S**2>=3.852
158A ->171A 0.11544
160A ->169A -0.24212
160A ->171A -0.13870
161A ->169A 0.19970
161A ->171A -0.11532
161A ->173A -0.10370
162A ->170A -0.13548
162A ->172A -0.24071
163A ->170A -0.15958
163A ->172A 0.21531
163A ->174A -0.18206
166A ->169A -0.25359
166A ->171A 0.12360
155B ->166B 0.13010
157B ->166B -0.23154
157B ->169B -0.17434
157B ->171B -0.19999
158B ->172B 0.13818
159B ->169B 0.27966

160B ->172B -0.22214
161B ->170B 0.16499
161B ->172B -0.20100
161B ->174B 0.17288
162B ->171B -0.12011

Excited State 59: 3.852-A 4.7013 eV 263.72 nm f=0.0176 <S**2>=3.460
158A ->168A 0.25598
159A ->167A -0.10789
160A ->168A 0.28109
160A ->170A 0.16429
160A ->172A 0.10007
160A ->174A 0.12262
161A ->170A -0.10858
161A ->172A 0.11236
161A ->174A -0.10642
162A ->167A -0.14281
162A ->169A 0.20699
162A ->171A -0.14473
162A ->173A -0.13962
163A ->169A -0.23959
165A ->169A -0.11693
166A ->172A -0.11190
154B ->165B 0.11275
157B ->167B 0.36904
157B ->170B 0.14475
157B ->172B 0.14111
158B ->169B -0.11158
158B ->171B 0.10463
159B ->170B -0.15780
159B ->174B -0.13259
160B ->169B 0.19745
160B ->171B -0.13538
161B ->168B -0.16529
161B ->169B 0.23128
162B ->167B 0.14173

Excited State 60: 3.866-A 4.7419 eV 261.46 nm f=0.0008 <S**2>=3.486
157A ->168A -0.24038
158A ->167A 0.28806
159A ->168A -0.19042
160A ->167A 0.18957

160A ->169A -0.15440
161A ->171A -0.11924
162A ->170A -0.15818
162A ->174A -0.14115
163A ->172A 0.13362
165A ->176A 0.12777
166A ->169A 0.43523
166A ->175A 0.12353
157B ->166B 0.28027
157B ->169B -0.15248
158B ->167B -0.14915
159B ->171B -0.17149
160B ->167B 0.13183
160B ->170B -0.13997
160B ->174B -0.11297
161B ->172B -0.14291
163B ->169B -0.10116
163B ->175B -0.10137
164B ->176B -0.10267

Excited State 61: 3.164-A 4.7465 eV 261.21 nm f=0.0773 <S**2>=2.252
157A ->167A 0.38031
158A ->168A -0.29201
159A ->167A 0.47102
156B ->166B 0.39940
158B ->168B -0.22672
160B ->168B 0.14211
161B ->168B -0.46608

Excited State 62: 3.735-A 4.7555 eV 260.72 nm f=0.0001 <S**2>=3.238
157A ->168A -0.27404
158A ->167A 0.50844
159A ->168A -0.33493
165A ->176A -0.33537
166A ->169A -0.29145
166A ->175A -0.33355
153B ->165B -0.11087
163B ->175B 0.26256
164B ->176B 0.26665

Excited State 63: 4.022-A 4.7567 eV 260.65 nm f=0.0006 <S**2>=3.795
157A ->167A 0.11568

158A ->168A -0.18193
159A ->167A 0.10508
164A ->176A 0.12812
165A ->169A 0.11567
165A ->175A 0.50092
166A ->176A 0.48897
163B ->176B -0.39259
164B ->175B -0.41026

Excited State 64: 3.868-A 4.7625 eV 260.34 nm f=0.0001 <S**2>=3.489
157A ->168A -0.15729
158A ->167A 0.36366
159A ->168A -0.26077
165A ->176A 0.36608
166A ->169A -0.29733
166A ->175A 0.37800
156B ->167B 0.10932
163B ->175B -0.30618
164B ->176B -0.30818

Excited State 65: 3.583-A 4.7629 eV 260.31 nm f=0.0197 <S**2>=2.960
157A ->167A -0.22133
158A ->168A 0.53073
159A ->167A -0.23017
164A ->168A 0.10666
165A ->169A 0.13533
165A ->175A 0.14139
166A ->176A 0.13698
154B ->165B -0.13499
154B ->167B 0.13007
156B ->166B 0.27453
157B ->167B -0.26959
158B ->168B -0.19302
160B ->168B 0.12264
161B ->168B -0.42379
162B ->167B -0.10205
163B ->176B -0.11574
164B ->175B -0.11819

Excited State 66: 3.607-A 4.7729 eV 259.76 nm f=0.0115 <S**2>=3.003
153A ->167A 0.13740
155A ->168A 0.14329

160A ->168A 0.10212
162A ->171A -0.10572
163A ->169A -0.10387
151B ->165B -0.11489
152B ->166B -0.12759
153B ->166B 0.11161
154B ->167B 0.14324
156B ->166B 0.44029
157B ->167B -0.17515
158B ->168B 0.17028
159B ->172B 0.10474
161B ->168B 0.51658
161B ->169B 0.12512
162B ->167B -0.19320

Excited State 67: 3.519-A 4.8044 eV 258.06 nm f=0.0002 <S**2>=2.845
153A ->168A -0.12630
154A ->167A -0.10536
155A ->167A -0.14739
157A ->168A 0.23270
158A ->167A 0.32277
161A ->169A 0.13864
162A ->172A -0.12630
165A ->170A 0.10142
166A ->169A 0.35876
166A ->171A -0.10070
152B ->165B 0.10909
153B ->165B -0.12702
154B ->166B 0.27387
155B ->166B -0.19511
157B ->166B 0.13070
159B ->168B 0.15819
159B ->169B 0.10157
162B ->166B -0.23040
162B ->168B 0.24644
163B ->169B 0.15277

Excited State 68: 3.539-A 4.8063 eV 257.96 nm f=0.0230 <S**2>=2.881
157A ->167A 0.18158
158A ->168A 0.36641
162A ->171A 0.12821
163A ->169A 0.13349

165A ->169A 0.19237
166A ->170A 0.19739
148B ->165B -0.19065
150B ->165B 0.16953
155B ->167B 0.11832
156B ->166B 0.25073
157B ->167B 0.48236
159B ->167B -0.10814
160B ->171B 0.12039
161B ->168B 0.31133
162B ->167B 0.13865

Excited State 69: 3.708-A 4.8191 eV 257.28 nm f=0.0058 <S**2>=3.187
153A ->168A 0.10615
157A ->168A -0.20242
159A ->168A -0.10009
160A ->167A -0.10415
160A ->171A -0.12115
161A ->169A 0.11674
162A ->170A 0.12841
162A ->172A -0.11050
162A ->174A 0.10331
163A ->170A -0.10171
163A ->172A -0.12525
166A ->169A 0.56902
166A ->173A -0.11185
155B ->166B 0.12541
156B ->167B -0.14746
157B ->166B -0.22599
157B ->169B 0.11212
159B ->168B -0.12446
159B ->171B 0.14757
160B ->170B 0.10320
161B ->172B 0.12260
162B ->166B 0.11244
162B ->168B -0.15637
163B ->169B 0.15401

Excited State 70: 3.320-A 4.8215 eV 257.15 nm f=0.2093 <S**2>=2.505
153A ->167A -0.11548
155A ->168A -0.12243
157A ->167A 0.18762

158A ->168A 0.25295
148B ->165B 0.41721
148B ->167B 0.23123
150B ->165B -0.38648
150B ->167B -0.20323
154B ->167B -0.23472
155B ->167B -0.24693
156B ->166B 0.24717
157B ->167B -0.16570
159B ->167B -0.11301
161B ->168B 0.12670

Excited State 71: 3.512-A 4.8367 eV 256.34 nm f=0.0030 <S**2>=2.833
153A ->167A 0.10935
155A ->168A 0.11217
157A ->167A -0.17284
158A ->168A -0.10474
165A ->169A 0.51538
166A ->170A -0.14167
166A ->172A 0.13311
148B ->165B 0.22721
148B ->167B 0.11744
150B ->165B -0.19168
150B ->167B -0.11490
151B ->165B -0.10225
155B ->167B -0.36404
157B ->167B 0.36530
159B ->167B -0.10043
161B ->168B -0.13716

Excited State 72: 3.256-A 4.8370 eV 256.32 nm f=0.0004 <S**2>=2.400
153A ->168A 0.11967
157A ->168A -0.18863
154B ->168B -0.13391
156B ->167B -0.12991
159B ->168B 0.59627
162B ->168B 0.62310
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 72 LETran= 1306.

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