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**Supplementary Information**

**An *in silico* design of antiviral nickel (II) complexes as therapeutic drug candidates**

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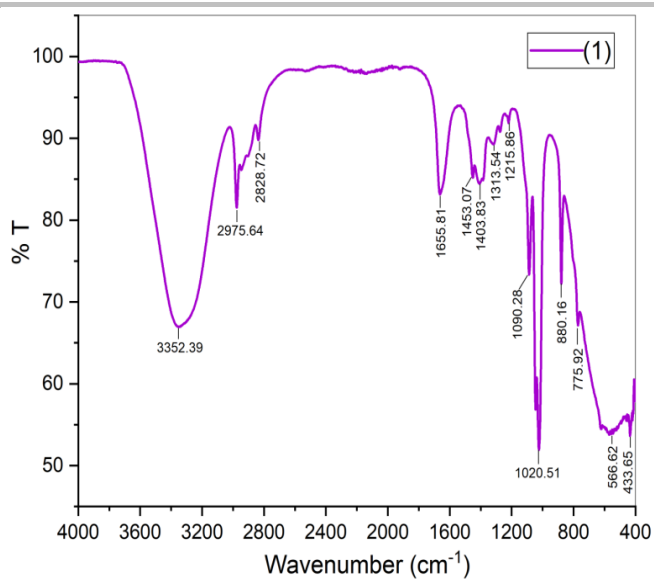
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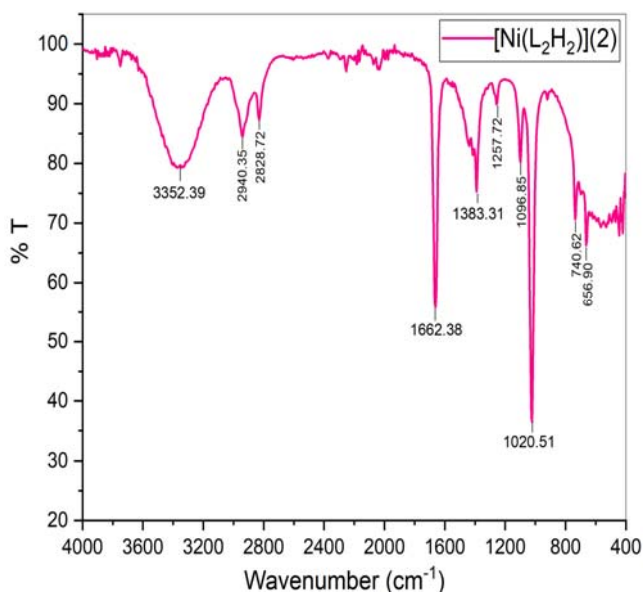
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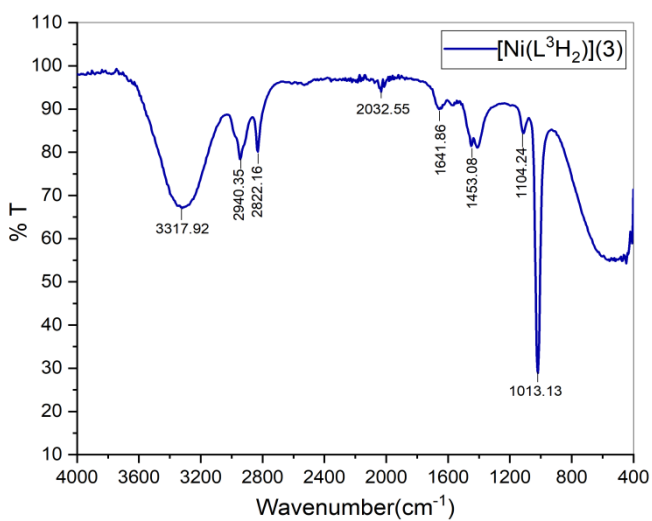
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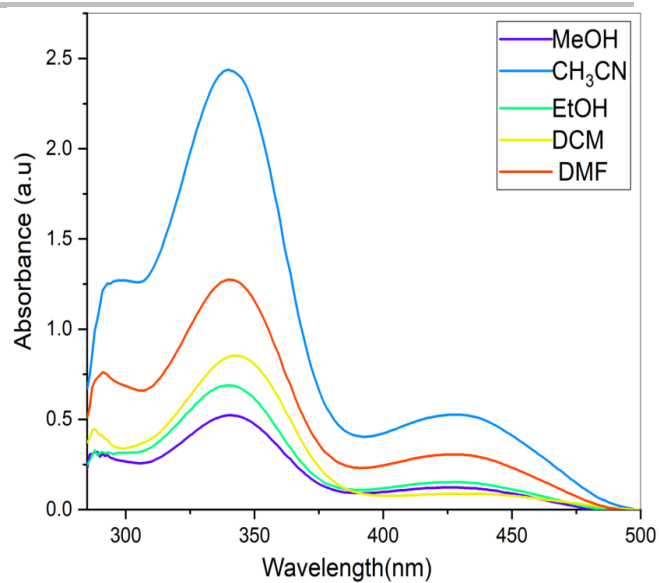
**Figure S1.** FT-IR spectra of nickel(II) complex  $[\text{Ni}(\text{L}^1)](1)$ .



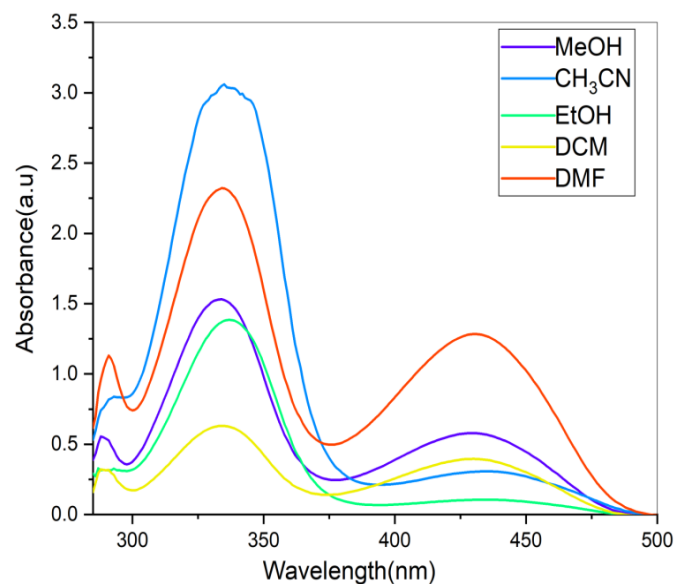
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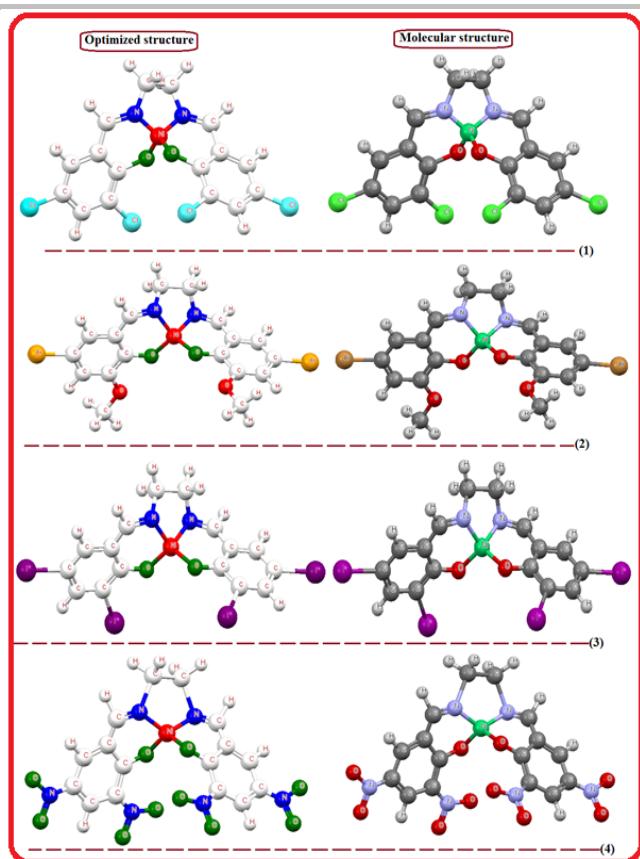
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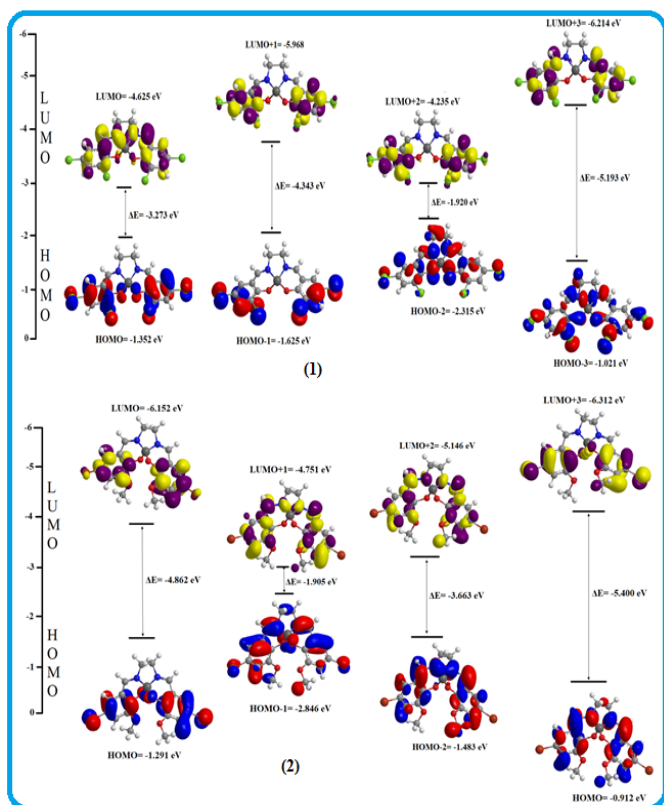
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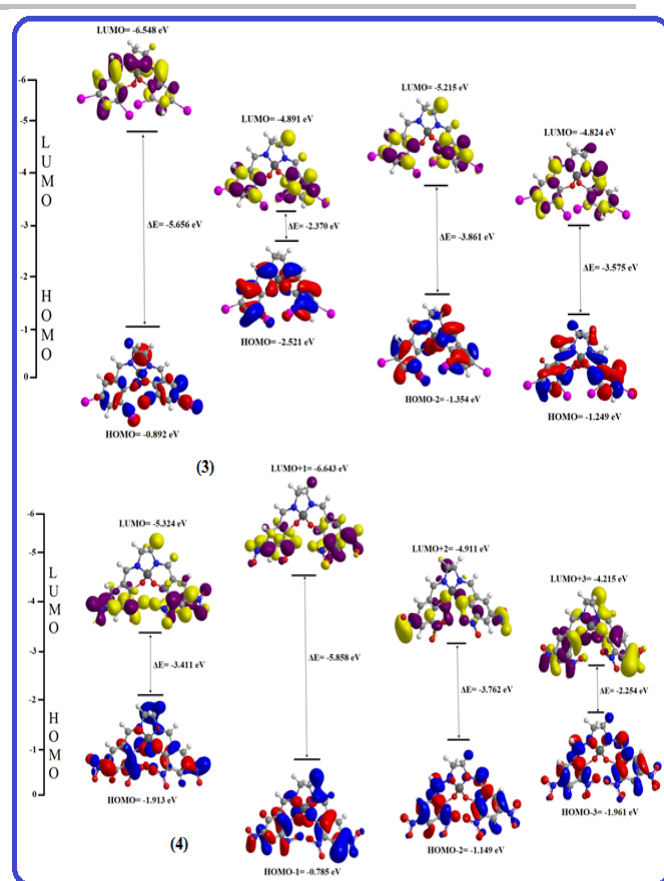
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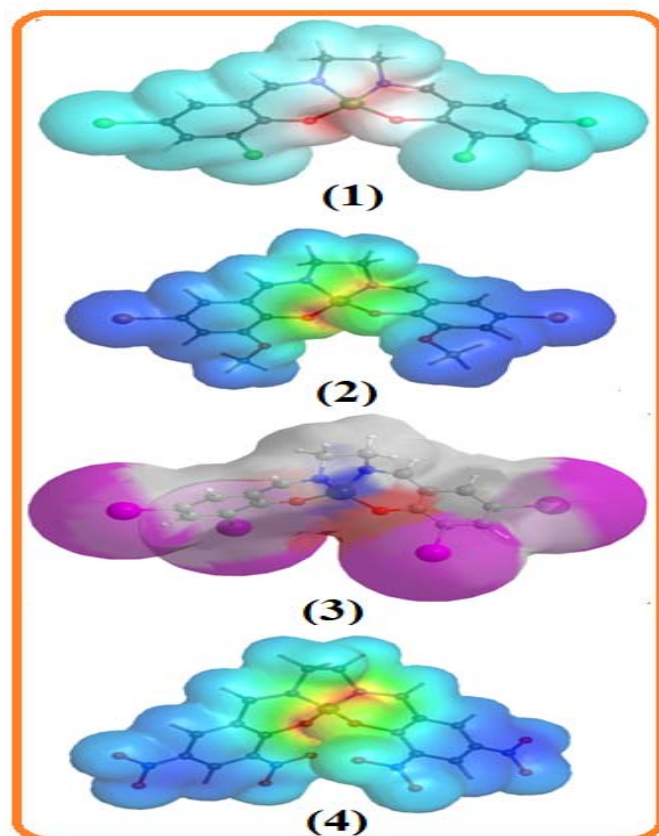
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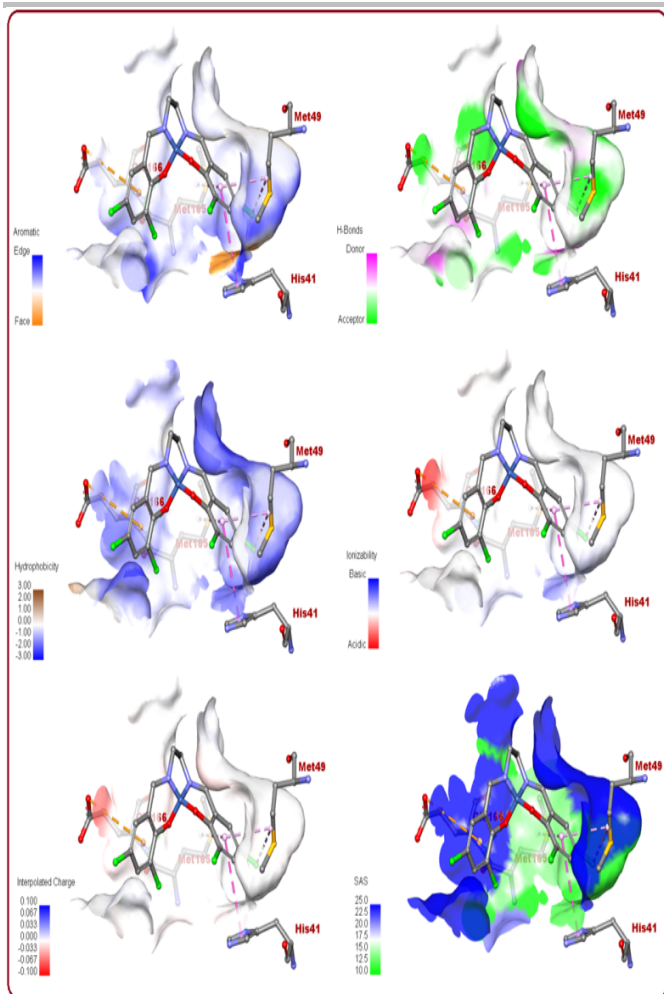
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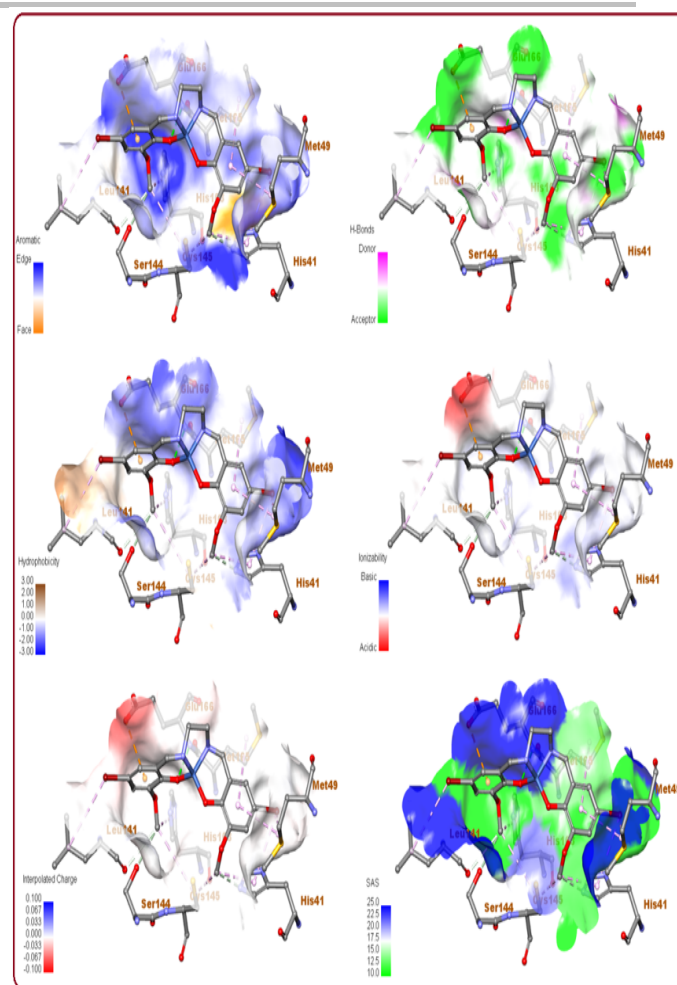
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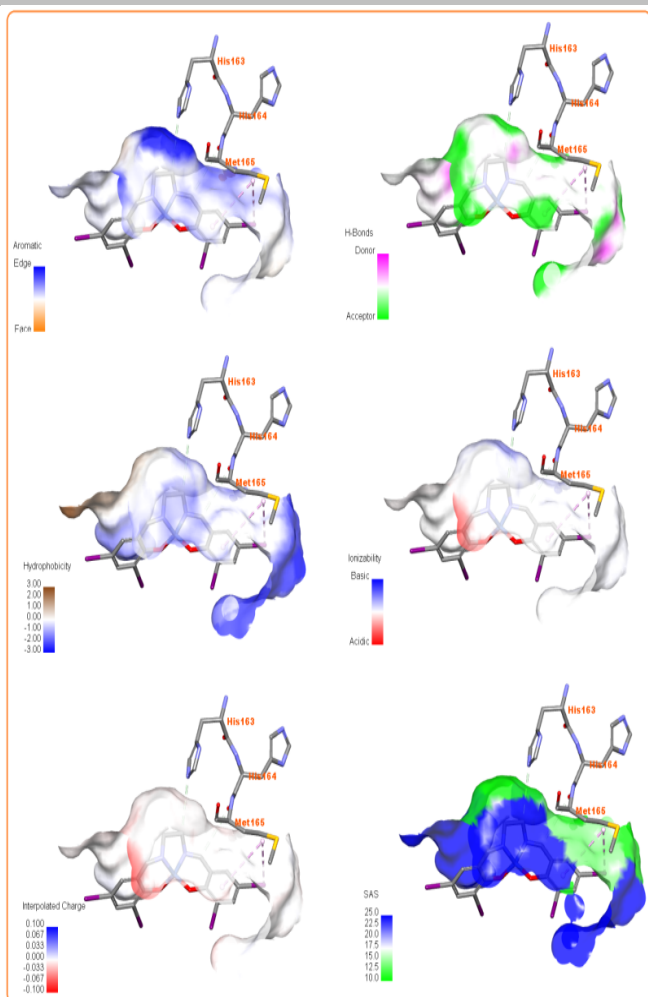
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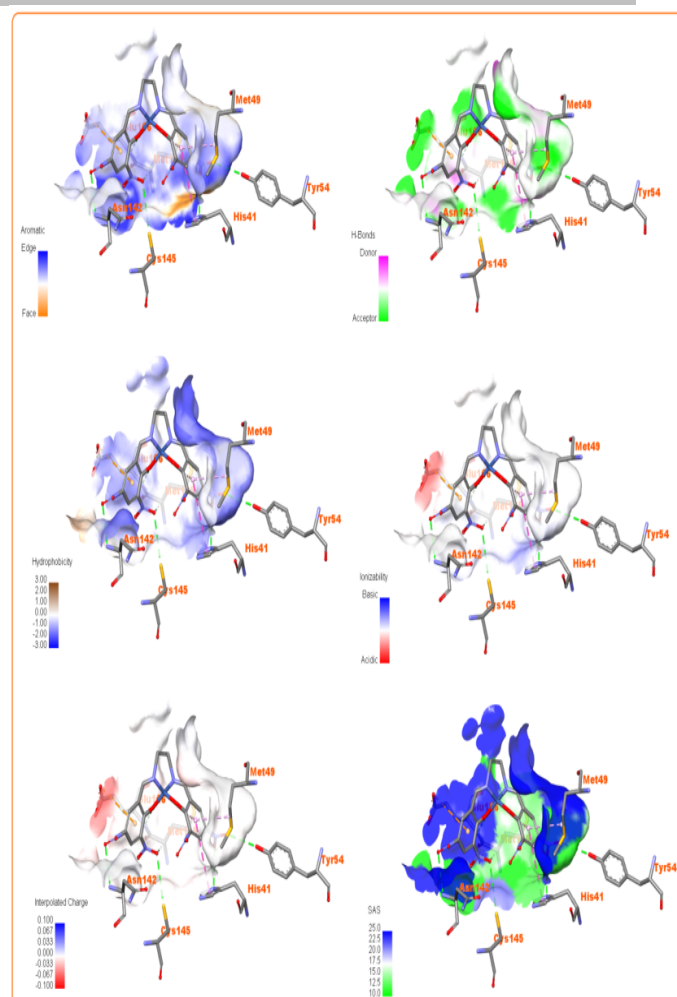
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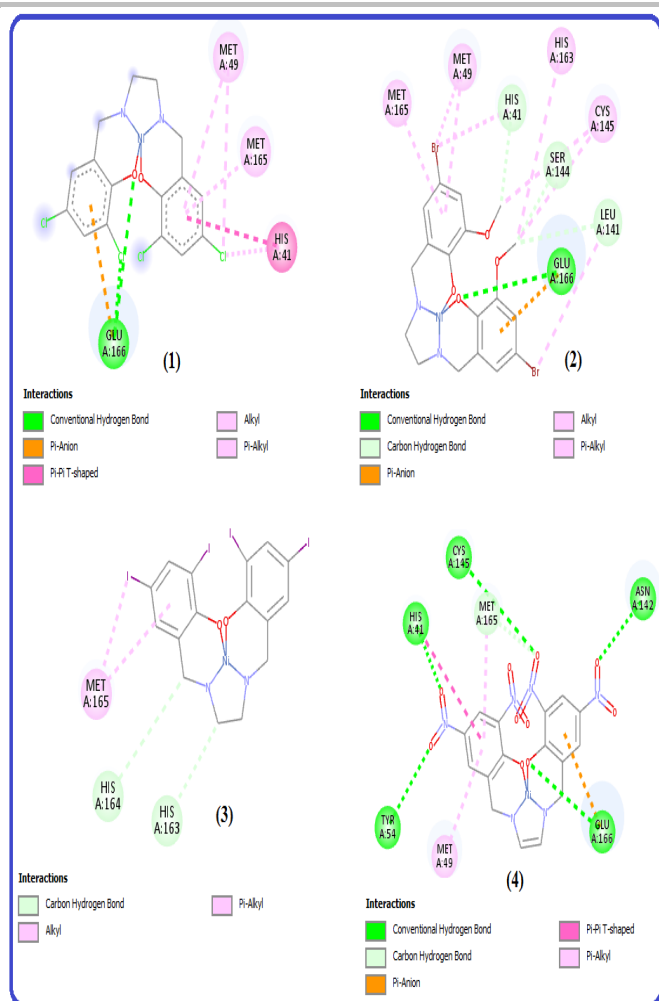
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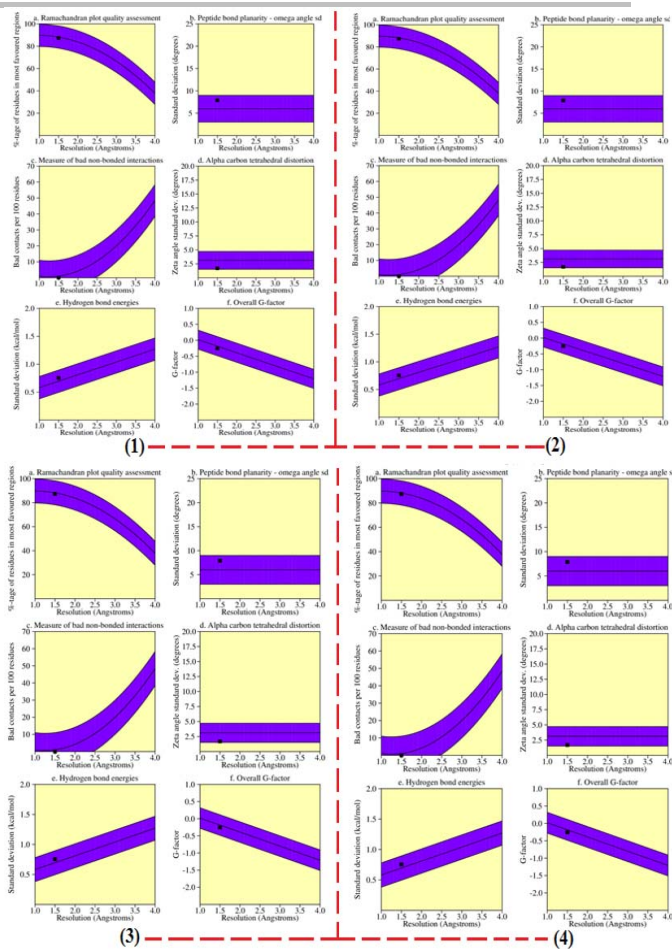
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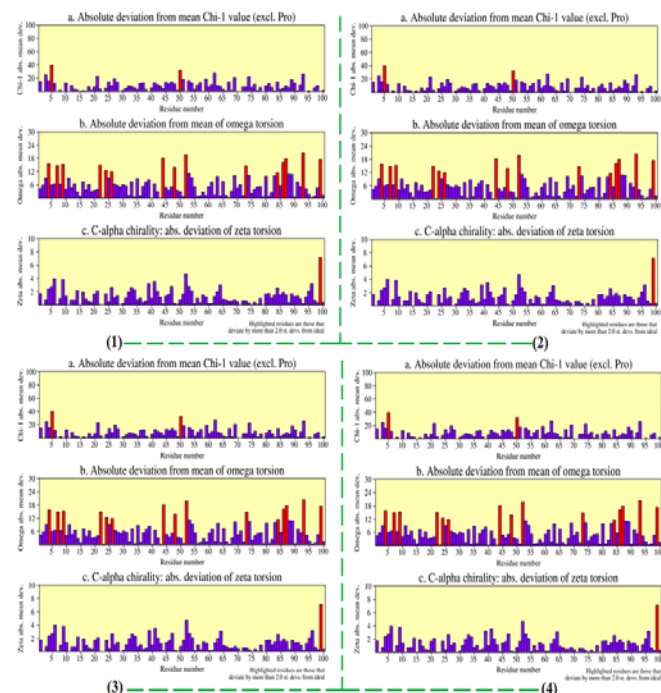
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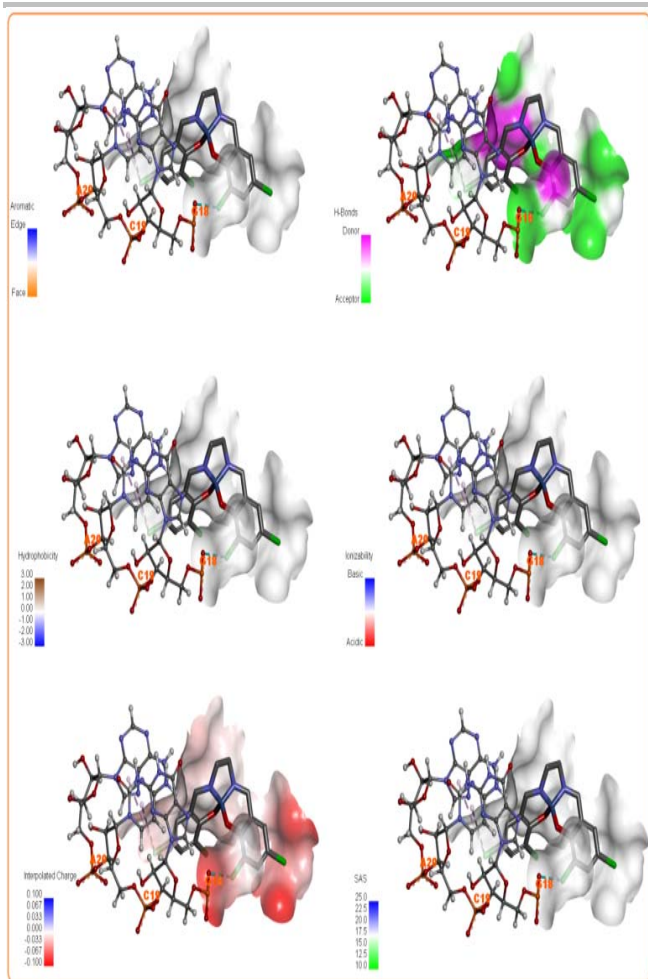
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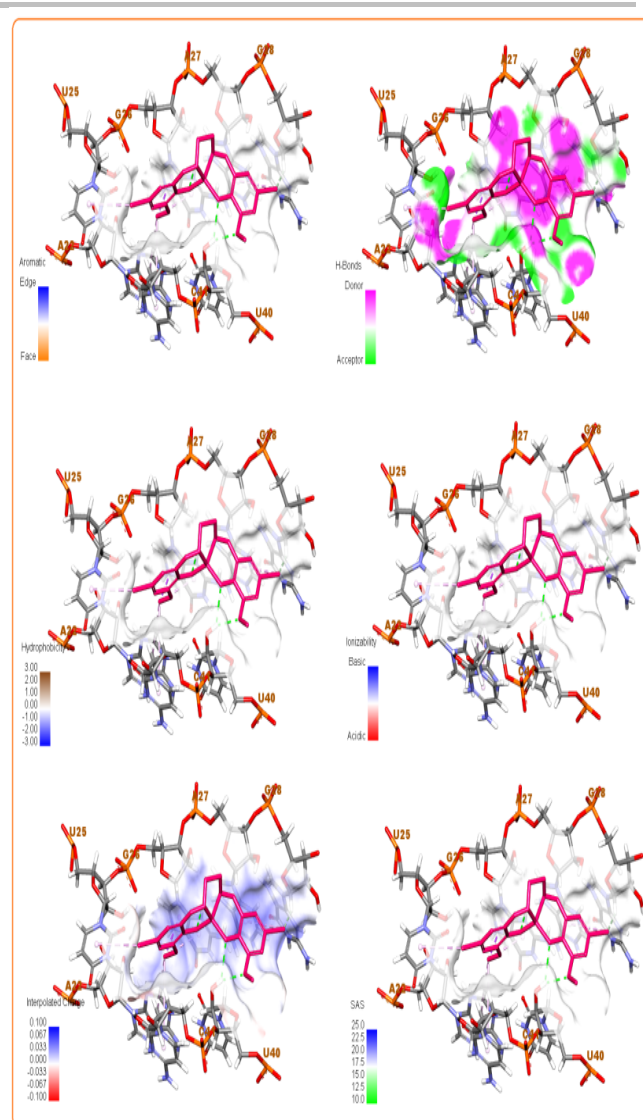
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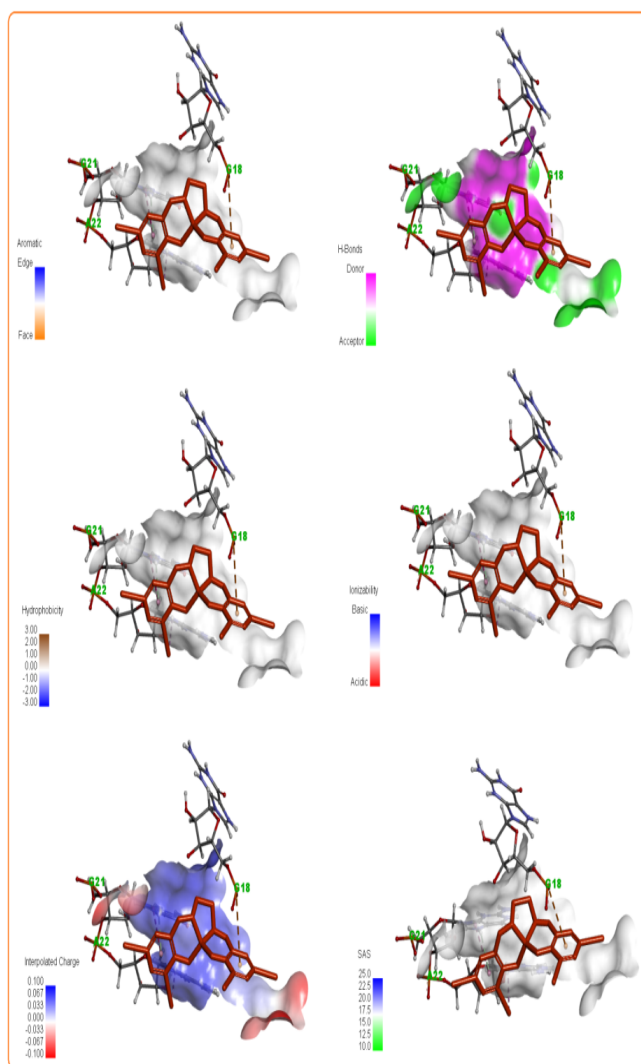
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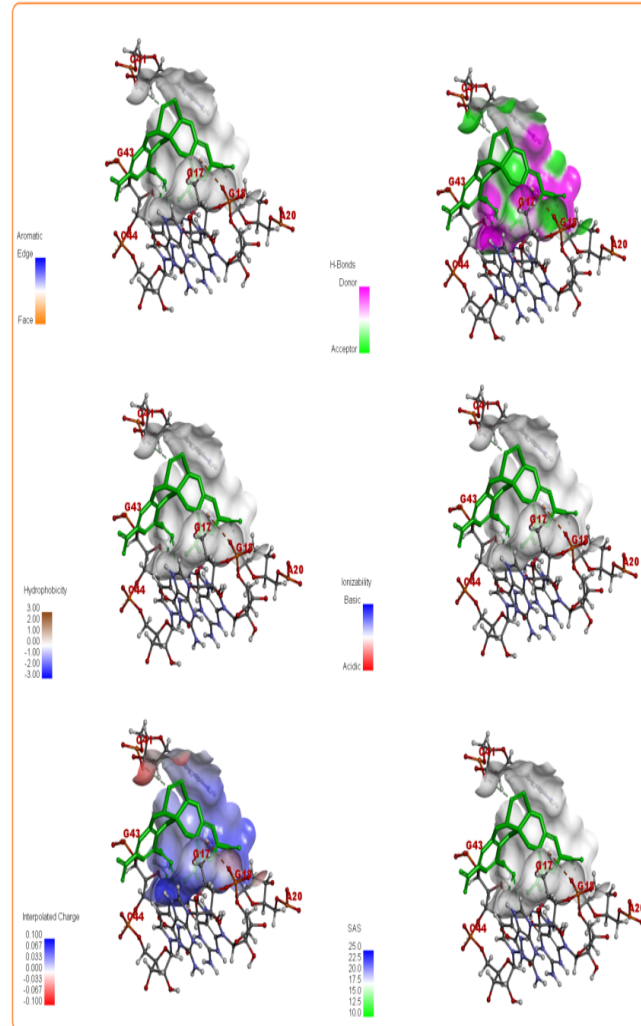
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**Figure S18.** The representation of docked nickel(II) complex  $[\text{Ni}(\text{L}^2)](2)$  with HIV-1 RNA (PDB ID: 1UUI) with its focused view for interacting residues along with H-bond and intermolecular interactions; (a) Aromatic receptor surface represented by blue (Edge) and light orange (face) colours; (b) H-bond donor and acceptor meshes represented by pink and light green colours, respectively; (c) Hydrophobic pocket represented with blue and brown colours; (d) ionizability receptor surface represented by blue (basic) and red (acidic) colours; (e) interpolated charge receptor surface represented by blue and red colours; (f) SAS receptor surface represented by blue and light green colours, respectively.



**Figure S19.** The representation of docked nickel(II) complex  $[\text{Ni}(\text{L}^3)](\mathbf{3})$  with HIV-1 RNA (PDB ID: 1UUI) with its focused view for interacting residues along with H-bond and intermolecular interactions; (a) Aromatic receptor surface represented by blue (Edge) and light orange (face) colours; (b) H-bond donor and acceptor meshes represented by pink and light green colours, respectively; (c) Hydrophobic pocket represented with blue and brown colours; (d) ionizability receptor surface represented by blue (basic) and red (acidic) colours; (e) interpolated charge receptor surface represented by blue and red colours; (f) SAS receptor surface represented by blue and light green colours, respectively.



**Figure S20.** The representation of docked nickel(II) complex  $[\text{Ni}(\text{L}^4)](\mathbf{4})$  with HIV-1 RNA (PDB ID: 1UUI) with its focused view for interacting residues along with H-bond and intermolecular interactions; (a) Aromatic receptor surface represented by blue (Edge) and light orange (face) colours; (b) H-bond donor and acceptor meshes represented by pink and light green colours, respectively; (c) Hydrophobic pocket represented with blue and brown colours; (d) ionizability receptor surface represented by blue (basic) and red (acidic) colours; (e) interpolated charge receptor surface represented by blue and red colours; (f) SAS receptor surface represented by blue and light green colours, respectively.

**Table S1.** Natural atomic charges on selected atoms of the nickel(II) complex  $[\text{Ni}(\text{L}^1)](\mathbf{1})$  using NBO analysis as calculated at the B3LYP/6-31G(d) level .

Atom	No	Charge
H	1	0.23521
H	2	0.25233
C	1	-0.27083
H	3	0.23078
H	4	0.22404
H	5	0.24183
C	2	-0.24589
H	6	0.23175

C	3	-0.24215
H	7	0.22481
O	1	-0.59614
C	4	-0.31422
C	5	-0.26024
C	6	0.34511
H	8	0.28144
C	7	0.27447
C	8	0.14877
H	9	0.23122
C	9	-0.32575
C	10	0.15677
O	2	-0.75422
N	1	-0.63008
C	11	-0.32290
C	24	-0.22023
N	2	-0.51811
C	12	-0.31584
C	13	0.36460
C	14	-0.25692
H	10	0.24819
C	15	0.24460
H	11	0.27184
H	12	0.24191
Ni	1	0.67870
H	13	0.19803
Cl	1	-0.0704
C	16	-0.21421
Cl	2	-0.0804

**Table S2.** Natural atomic charges on selected atoms of the nickel(II) complex [Ni(L<sup>2</sup>)] (2) using NBO analysis as calculated at the B3LYP/6-31G(d) level.

Atom	No	Charge
H	1	0.23221
H	2	0.24333
C	1	-0.25087
H	3	0.24078
H	4	0.22412
H	5	0.24512
C	2	-0.24565
H	6	0.22174
C	3	-0.24612
H	7	0.22491
O	1	-0.59685
C	4	-0.32369
C	5	-0.29214
C	6	0.32345
H	8	0.27451
C	7	0.24258
C	8	0.16234
H	9	0.23487
C	9	-0.33512
C	10	0.16214
O	2	-0.72145
N	1	-0.61258
C	11	-0.36321
C	24	-0.22152
N	2	-0.52345
C	12	-0.32147
C	13	0.36514
C	14	-0.25459
H	10	0.24540
C	15	0.24591
H	11	0.26158
H	12	0.24257
Ni	1	0.67891
H	13	0.19426
C	16	-0.21891
Br	1	-0.08521

**Table S3.** Natural atomic charges on selected atoms of the [Ni(L<sup>3</sup>)] (3) using NBO analysis as calculated at the B3LYP/6-31G(d) level .

Atom	No	Charge
H	1	0.23841
H	2	0.25542
C	1	-0.27183
H	3	0.22074
H	4	0.22128
H	5	0.23581
C	2	-0.25624
H	6	0.24187
C	3	-0.24612
H	7	0.22814
O	1	-0.59148
C	4	-0.31214
C	5	-0.26517
C	6	0.34412
H	8	0.28283
C	7	0.27813
C	8	0.14814
H	9	0.23231
C	9	-0.32412
C	10	0.15412
O	2	-0.77419
N	1	-0.63142
C	11	-0.35521
C	17	-0.23841
N	2	-0.52418
C	12	-0.32614
C	13	0.35640
C	14	-0.26248
H	10	0.24421
C	15	0.23658
H	11	0.27484
H	12	0.24294
Ni	1	0.64941
H	12	0.18943
I	1	-0.06315
C	16	-0.21312
I	2	-0.06716

**Table S4.** Natural atomic charges on selected atoms of the nickel(II) complex [Ni(L<sup>4</sup>)] (4) using NBO analysis as calculated at the B3LYP/6-31G(d) level .

Atom	No	Charge
H	1	0.23657
H	2	0.25633
C	1	-0.28062
H	3	0.24032
H	4	0.23021
H	5	0.24425
C	2	-0.24689
H	6	0.23784
C	3	-0.24351
H	7	0.22478
O	1	-0.59746
C	4	-0.31562
C	5	-0.26185
C	6	0.34921
H	8	0.28245
C	7	0.27561
C	8	0.14864
H	9	0.23253
C	9	-0.32472

C 10 0.15244  
 O 2 -0.74512  
 N 1 -0.61348  
 C 11 -0.33627  
 C 17 -0.24025  
 N 2 -0.51749  
 C 12 -0.32150  
 C 13 0.36122  
 C 14 -0.25495  
 H 10 0.24981  
 C 15 0.24562  
 H 11 0.27184  
 H 12 0.24927  
 Ni 1 0.66120  
 N 3 -0.52514  
 O 3 -0.77412  
 O 4 -0.75358  
 H 13 0.19514  
 C 16 -0.21458

**Table S6.** The geometrical parameters of optimized ground-state geometry for the Ni(II) complexes (1)-(4) calculated through the B3LYP/6-31G(d) level .

Complex [Ni(L <sup>1</sup> )] (1)		Complex [Ni(L <sup>2</sup> )] (2)		Complex [Ni(L <sup>3</sup> )] (3)		Complex [Ni(L <sup>4</sup> )] (4)	
Ni(1)-O(1)	1.770	Ni(1)-O(1)	1.769	Ni(1)-O(1)	1.769	Ni(1)-O(1)	1.773
Ni(1)-O(2)	1.771	Ni(1)-O(2)	1.768	Ni(1)-O(2)	1.767	Ni(1)-O(2)	1.771
Ni(1)-N(1)	1.812	Ni(1)-N(1)	1.809	Ni(1)-N(1)	1.809	Ni(1)-N(1)	1.824
Ni(1)-N(2)	1.813	Ni(1)-N(2)	1.808	Ni(1)-N(2)	1.806	Ni(1)-N(2)	1.805
C(2)-Cl(1)	1.719	C(4)-Br(1)	1.895	C(2)-I(1)	2.160	C(2)-N(3)	1.306
C(4)-Cl(2)	1.720	C(2)-O(3)	1.409	C(4)-I(2)	2.174	C(4)-N(5)	1.263

**Table S5.** Summary of natural atomic charges and electron configuration (NEC) of the nickel (II) complexes (1)-(4) calculated through at the B3LYP/6-31G(d) level .

Nickel (II) complex [Ni(L <sup>1</sup> )] (1)		
O 1	-0.53511	[core] 2S (1.56)2p (4.89)3p (0.01)
O 2	-0.55122	[core] 2S (1.55)2p (4.89)3p (0.01)
N 1	-0.52102	[core] 2S (1.28)2p (4.32)3p (0.01)
N 2	-0.52211	[core] 2S (1.28)2p (4.32)3p (0.01)
O 3	-0.66664	[core] 2S (1.59)2p (5.15)3p (0.01)
O 4	-0.66662	[core] 2S (1.59)2p (5.15)3p (0.01)
Ni 1	0.66478	[core]4S( 0.34)3d( 7.55)4p( 0.42)4d( 0.03)5d( 0.05)
Nickel (II) complex [Ni(L <sup>2</sup> )] (2)		
O 1	-0.52411	[core] 2S (1.55)2p (4.87)3p (0.01)
O 2	-0.53522	[core] 2S (1.57)2p (4.89)3p (0.01)
N 1	-0.52202	[core] 2S (1.26)2p (4.32)3p (0.01)
N 2	-0.52411	[core] 2S (1.27)2p (4.32)3p (0.01)
O 3	-0.65664	[core] 2S (1.58)2p (5.15)3p (0.01)
O 4	-0.65662	[core] 2S (1.59)2p (5.15)3p (0.01)
Ni 1	0.65478	[core]4S( 0.32)3d( 7.45)4p(0.41)4d( 0.03)5d( 0.05)
Nickel (II) complex [Ni(L <sup>3</sup> )] (3)		
O 1	-0.52352	[core] 2S (1.58) 2p (4.82) 3p (0.01)
O 2	-0.52522	[core] 2S (1.58)2p (4.82)3p (0.01)
N 1	-0.53302	[core] 2S (1.29)2p (4.32)3p (0.01)
N 2	-0.52611	[core] 2S (1.29)2p (4.31)3p (0.01)
O 3	-0.64664	[core] 2S (1.56)2p (5.13)3p (0.01)
O 4	-0.64662	[core] 2S (1.56)2p (5.13)3p (0.01)
Ni 1	0.65678	[core]4S( 0.32)3d( 7.49)4p(0.43)4d( 0.03)5d( 0.05)
Nickel (II) complex [Ni(L <sup>4</sup> )] (4)		
O 1	-0.52142	[core] 2S (1.57) 2p (4.86) 3p (0.01)
O 2	-0.52142	[core] 2S (1.57)2p (4.86)3p (0.01)
N 1	-0.53602	[core] 2S (1.31)2p (4.24)3p (0.01)
N 2	-0.53603	[core] 2S (1.31)2p (4.24)3p (0.01)
O 3	-0.61564	[core] 2S (1.59)2p (5.16)3p (0.01)
O 4	-0.61562	[core] 2S (1.58)2p (5.16)3p (0.01)
Ni 1	0.63778	[core]4S( 0.34)3d( 7.52)4p(0.41)4d( 0.03)5d( 0.05)