

Supporting Information

Controlled Protein Dimerization through Hybrid Metal Coordination Motifs

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Section S1. Experimental Figures

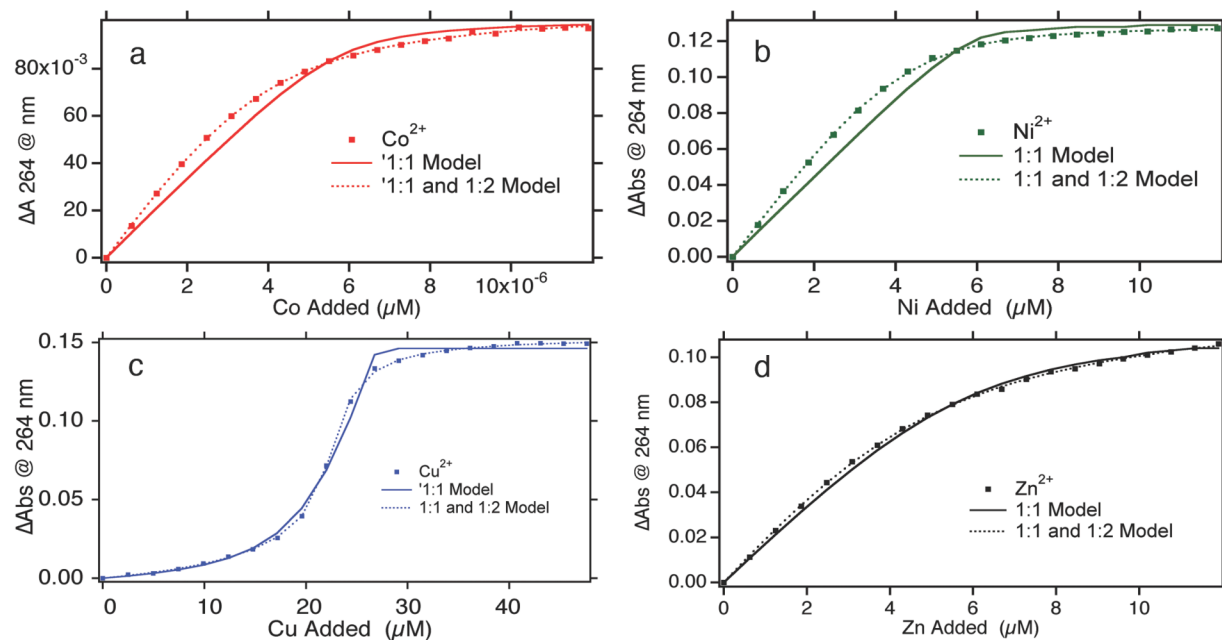


Figure S1.1. Metal binding titration data and fits for AQuin1. The lower metal affinity of AQuin1 (compared to HQuin1) allows for spectral changes due to M^{2+} ((a) Co^{2+} (b) Ni^{2+} (d) Zn^{2+}) binding to be directly monitored without the need for a competing ligand. Regression analysis for Co, Ni and Zn binding was performed assuming both a simple 1:1 (solid) and 1:1/1:2 (dotted line) binding event. The notable exception is (c) Cu binding, for which the dissociation constant is still low enough to require both the inclusion of EGTA as a competing ligand AQuin1 concentrations ranged from 2 to 10 μM , and EGTA concentration was 25 μM for the Cu^{2+} titration.

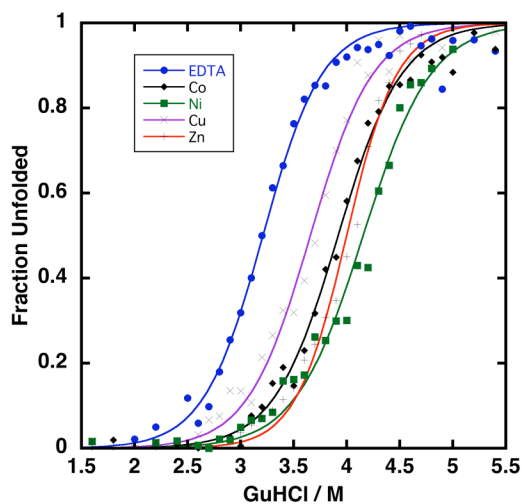


Figure S1.2. GuHCl unfolding data and fits for HQuin1 in the presence EDTA (blue), Co^{2+} (black), Ni^{2+} (green), Cu^{2+} (purple) and Zn (red). The parameters obtained from the fits are listed in Table S3.4.

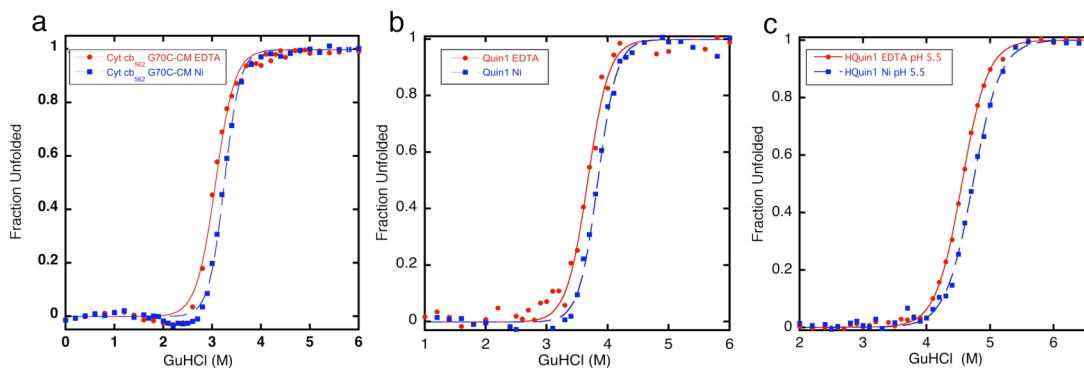


Figure S1.3. GuHCl unfolding titrations and fits for cyt cb_{562} variants in the absence (■) and presence of 1 mM Ni^{2+} (●). (a) (CM)-G70C-cyt cb_{562} in 100 mM Tris buffer (pH 7.5) (b) Aquin1 in 100 mM Tris buffer (pH 7.5) (c) HQuin1 in 100 mM sodium acetate buffer (pH 5.5). Fitting parameters and statistics are listed in Table S3.4.

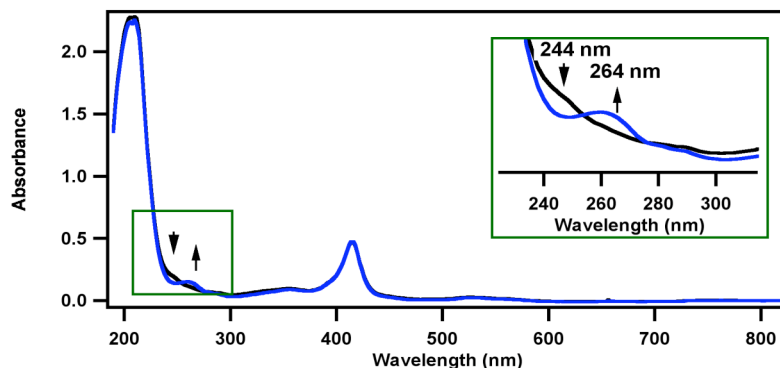


Figure S1.4. UV-visible spectra of HQuin1 in 100 mM sodium acetate (pH 5.5) with either 1 mM EDTA (black) or 1 mM Ni^{2+} (Blue). (Inset) The change in absorbance of the Quin group from the metal-free form ($\lambda_{max}=244$ nm) to the metal bound form ($\lambda_{max}=264$ nm) indicates the Quin group retains its ability to bind metal even though no protein stabilization is observed at pH 5.5 (see Figure S2.4c).

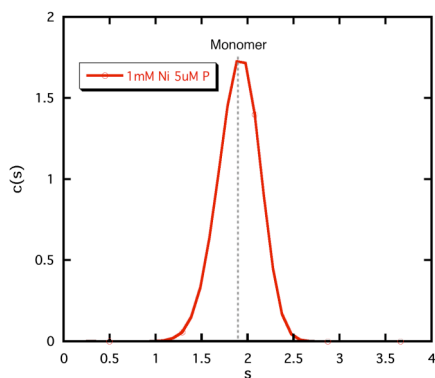


Figure S1.5. Sedimentation coefficient distribution for HQuin1 under identical solution conditions as the unfolding titrations (5 μ M HQuin1, 1 mM Ni^{2+} in 100 mM Tris (pH 7)). This experiment reveals that HQuin1 remains monomeric during unfolding titrations.

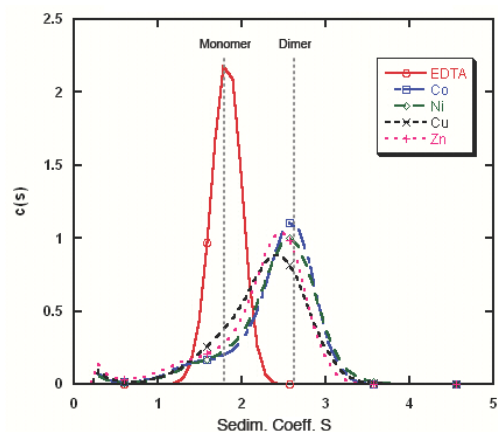


Figure S1.6. Sedimentation coefficient distributions of HQin1 (25 μM) in the presence of 1 mM EDTA (red) or 12.5 μM M^{2+} : Co (blue), Ni (green), Cu (black), Zn (pink). Experiments were conducted at 25°C.

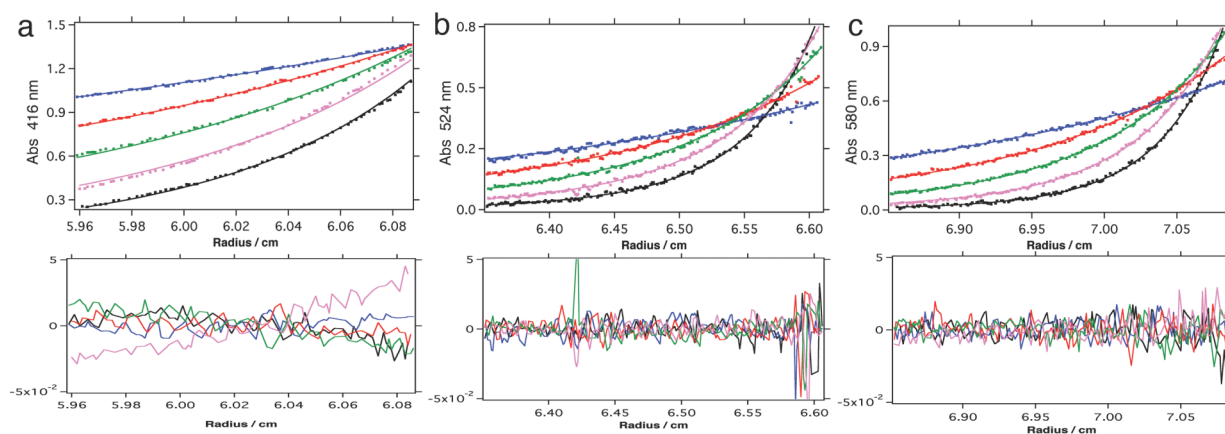


Figure S1.7. Sedimentation equilibrium profiles for HQin1 in the presence of Ni^{2+} . (a) 5 μM protein at 15,000 (blue), 20,000 (red), 25,000 (green), 30,000 (pink) and 35,000 (black) rpm. (b) 25 μM protein at 15,000 (blue), 20,000 (red), 25,000 (green), 30,000 (pink) and 35,000 rpm (black). (c) 200 μM protein at 15,000 (blue), 20,000 (red), 25,000 (green), 30,000 (pink) and 35,000 rpm (black). All samples were in 20 mM TRIS buffer (pH 7) with a half equivalent of NiSO_4 . Scans shown in a), b) and c) were globally fit to a monomer-dimer model yielding a minimized fit with a $\log K^{\text{Dimer}} = 4.38 \pm 0.023 \text{ M}^{-1}$ or $K_D^{\text{dimer}} = 41.6(2) \mu\text{M}$. Experiments were conducted at 25°C.

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e = 1e-4 ?
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pm + p <=> d: kd3 dissociation
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d = 4e4 ?
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Figure S1.8. Example DynaFit scripts used for fitting HQuin1 and AQuin1 metal binding titrations. (a) 1:1 competitive binding model, (b) 1:1/1:2 competitive binding model, (c) 1:1 binding model and (d) 1:1/1:2 binding models. All models include the following variables: free protein (p), free metal (m), metal-bound protein (pm). Variables for the concentration of free EGTA (e), EGTA-metal complex (em) and metal-induced metal dimer (d) were included where appropriate. The following dissociation constants were determined by non-linear regression analysis: kd1 (for initial protomer-metal binding), and kd3 (metal-induced dimerization). The metal dissociation constants for EGTA (kd2) were calculated using Maxchelator and held fixed. Values associated with “?” signify that the value was allowed to float during the fitting process.

Section S2. Experimental Tables

Metal	K_D^{metal} (M)	K_D EGTA (M)
Co ²⁺	$4.0(2) \times 10^{-9}$	9.68×10^{-9}
Ni ²⁺	$4.0(2) \times 10^{-10}$	5.80×10^{-10}
Cu ²⁺	$8.5(9) \times 10^{-14}$	4.21×10^{-14}
Zn ²⁺	$7.1(3) \times 10^{-9}$	5.26×10^{-9}

Table S2.1. Fitting parameters for metal binding titrations of HQuin1. Data fit using a 1:1 model. In all cases EGTA was used as competing ligand. EGTA:metal dissociation constants were determined using Maxchelator (<http://maxchelator.stanford.edu>) (25° C and a ionic strength of 0.05 M) and were held fixed during regression analysis.

Metal	K_D^{metal} (M)	K_D^{dimer} (M)	K_D EGTA (M)
Co ²⁺	$2(3) \times 10^{-8}$	$2(3) \times 10^{-6}$	9.68×10^{-9}
Ni ²⁺	$8.3(8) \times 10^{-10}$	$6(9) \times 10^{-4}$	5.80×10^{-10}
Cu ²⁺	$2(10) \times 10^{-12}$	$1(6) \times 10^{-6}$	4.21×10^{-14}
Zn ²⁺	$3(16) \times 10^{-9}$	$3(14) \times 10^{-6}$	5.26×10^{-9}

Table S2.2. Fitting parameters for metal binding titrations of HQuin1 fit using a 1:1/1:2 (the latter representing protein dimerization) model.

Metal	K_D^{metal} (M)
Co ²⁺	$2(1) \times 10^{-7}$
Ni ²⁺	$4(5) \times 10^{-8}$
Cu ²⁺	$6.0(1) \times 10^{-13}$
Zn ²⁺	$6(1) \times 10^{-7}$

Table S2.3. Fitting parameters for metal binding titrations of AQuin1. Data were fit using a 1:1 model and determined via direct titration.

Metal	K_D^{metal} (M)	K_D^{dimer} (M)
Co ²⁺	$3.0(1) \times 10^{-7}$	$2(1) \times 10^{-6}$
Ni ²⁺	$3(1) \times 10^{-8}$	$9(5) \times 10^{-7}$
Cu ^{2+*}	$5.4(5) \times 10^{-9}$	$6.0(4) \times 10^{-9}$
Zn ²⁺	$9(1) \times 10^{-7}$	$6(3) \times 10^{-6}$

Table S2.4. Fitting parameters for metal binding titrations of AQuin1. Data was fit using a 1:1/1:2 (the latter representing protein dimerization) model and determined via direct titration method. *Dissociation constants determined via competition assay using 25 μ M EGTA as competing ligand.

cyt <i>cb</i> ₅₆₂ variant	Condition	Slope, m_1 (kcal/mol•M)	[GuHCl] _m , m_2 (M)	Figure
HQuin1	EDTA	2.1(1)	3.21(2)	1A, S2.4
HQuin1	Co	1.9(7)	3.91(1)	S2.4
HQuin1	Ni	1.8(8)	4.15(1)	1A, S2.4
HQuin1	Cu	1.9(1)	3.66(1)	S2.4
HQuin1	Zn	2.4(1)	3.99(1)	S2.4
(CM)-G70C	EDTA	2.9(1)	3.06(1)	S2.5a
(CM)-G70C	Ni	3.6(1)	3.24(1)	S2.5a
AQuin1	EDTA	3.4(2)	3.66(1)	S2.5b
AQuin1	Ni	3.8(2)	3.83(1)	S2.5b
HQuin1	EDTA (pH 5.5)	2.9(6)	4.55(1)	S2.5c
HQuin1	Ni (pH 5.5)	2.7(1)	4.73(1)	S2.5c

Table S2.5. Fitting parameters for chemical unfolding titrations of cyt *cb*₅₆₂ variants: HQuin1, AQuin1, (CM)-G70C cyt *cb*₅₆₂.

HQuin1	T _m (K)	slope (kcal/mol)	Figure
EDTA	337(1)	100(20)	1B
Ni	349(1)	55(4)	1B

Table S2.6. Fitting parameters for thermal unfolding titrations of HQuin1 (Figure 1B).

Contents of the asymmetric unit	106 residues + 1 Heme + 1 5-acetamide-8-hydroxyquinoline + 0.5 Ni + 46 waters
Unit cell dimensions	a = 88.44 Å , b = 34.51 Å, c = 46.90 Å $\alpha = \beta = \gamma = 90^\circ$
Symmetry group	<i>P2₁2₁2</i>
Resolution (Å)	50-2.30
X-ray wavelength (Å)	1.54
Number of Unique Reflections	6761
Redundancy	5.0 (3.2)
Completeness (%) [*]	99.0 (95.5)
$\langle I / \sigma I \rangle$ [*]	14.3 (2.3)
$R_{\text{sym}}^{\ddagger}$ (%) [*]	6.5 (40.9)
R^{\S} (%) [*]	26.6 (34.7)
Free R^{II} (%) [*]	31.4 (39.4)
Rms Bnd [¶] (Å)	0.014
Rms Ang [¶] (°)	1.21
Ramachandran plot (%)	
Residues in most favored regions	90.8
Residues in add.l allowed regions	9.2
Residues in generously allowed regions	0.0
Residues in disallowed regions	0.0

Table S2.7. X-ray data collection and refinement statistics for Ni:HQuin1.

$$\ddagger R_{\text{sym}} = \frac{\sum \sum_j |I_j - \langle I \rangle|}{\sum \sum_j I_j}$$

$$\S R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum F_{\text{obs}}}$$

^{II}Free R calculated against 7.4 of the reflections removed at random.

[¶]Root mean square deviations from bond and angle restraints.

^{*}Numbers in parentheses correspond to the highest resolution shell (2.39-2.30 Å)

Model	Total Bonding Energy (kcal mol ⁻¹)	ΔE (kcal mol ⁻¹)
<i>cis</i>-Quin BP86	-9438.29	6.08
<i>trans</i> -Quin BP86	-9432.21	
<i>cis</i>-Quin OLYP	-9185.43	5.21
<i>trans</i> -Quin OLYP	-9180.22	

Table S2.8. Total bonding energies for geometry optimized models. Lowest energy isomer and corresponding total bonding energy are in bold. $\Delta E = |trans \text{ isomer} - cis \text{ isomer}|$.

Section S3. Input Files For Density Functional Calculations

S3.1. Input file for cis-Quin BP86

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XC  
LDA VWN  
GGA Becke Perdew  
END  
  
SYMMETRY NOSYM  
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H	-3.77036862	1.14378537	4.77676581
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H	-1.23722323	2.41056410	2.17819989
H	1.95229620	-2.42859631	3.31982008
H	3.56462245	-1.24309972	4.76155725
H	3.86968030	3.13203658	3.01090361
H	2.77522390	4.27533838	1.10830181
H	1.11821456	3.09248173	-0.28241603
H	0.00718995	3.09654594	-1.17480704
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H	-2.82978431	2.73157487	-4.37486370
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H	-2.93414546	-2.76332242	-2.25634490
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H	3.88318285	-1.40365048	-4.65062009
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H	1.61729250	-2.46365419	-0.31429527
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core none
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END INPUT"

S3.3. Input file for *cis*-Quin OLYP

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MAXMEMORYUSAGE 7000

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END

XC
GGA OLYP
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SYMMETRY NOSYM
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5.C	3.067748	-1.211423	-2.947351
6.C	2.005525	1.580376	-0.626074
7.C	3.853038	1.168788	-2.829998
8.C	3.043509	0.087600	-2.381129
9.C	2.129828	0.305133	-1.300534
10.N	1.305921	-0.681032	-0.855962
11.N	4.730897	0.966737	-3.939152
12.O	1.184926	1.701304	0.390447
13.C	2.437509	-2.921593	4.885147
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18.N	1.223016	-0.765627	2.083426
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20.C	-1.351280	1.888106	-1.400375
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22.C	-3.702722	-2.393864	-2.231841
23.C	-3.058864	1.218246	-2.957816
24.C	-2.014977	-1.583542	-0.640540
25.C	-3.852034	-1.160544	-2.850865
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31.Ni	-0.013287	-0.005522	0.576671
32.C	-2.427966	2.938778	4.892530
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34.C	-1.180547	1.961229	2.782162
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36.C	-2.087768	-0.007876	2.742510
37.N	-1.214771	0.756352	2.110500
38.H	2.246748	-3.204075	-2.869882
39.H	0.667883	-2.626945	-0.986157
40.H	2.726432	3.605812	-0.691999
41.H	4.304043	3.239884	-2.555113
42.H	3.722499	-1.414158	-3.794235
43.H	5.203585	1.831942	-4.193106
44.H	5.443249	0.261482	-3.746542
45.H	3.191272	-2.508255	5.568697
46.H	1.569987	-3.213524	5.492666
47.H	2.859985	-3.835468	4.446808
48.H	0.543447	-2.769587	2.440290
49.H	3.318641	-0.290485	4.410766
50.H	2.346571	1.016193	2.412637
51.H	-2.229077	3.207099	-2.872524
52.H	-0.653711	2.616459	-0.990083
53.H	-2.740579	-3.607140	-0.715761
54.H	-4.311256	-3.230525	-2.582830
55.H	-3.712952	1.427587	-3.803558
56.H	-5.210097	-1.812993	-4.211642
57.H	-5.435512	-0.240471	-3.765605
58.H	-3.184399	2.533601	5.578505
59.H	-1.563133	3.239026	5.499372

60.H	-2.849143	3.847595	4.441786
61.H	-0.532818	2.762715	2.448374
62.H	-3.307134	0.302855	4.445567
63.H	-2.344242	-1.019720	2.454838

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core none
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END INPUT"

S3.4. Input file for *trans*-Quin OLYP

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MAXMEMORYUSAGE 7000

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3.C      2.257117   -1.394138    3.241701
4.C      3.190055   -0.752434    4.067420
5.C      3.266868    2.666845    2.550695
6.C      1.637437   -0.725907    2.166684
7.C      3.566179    0.574659    3.901047
8.C      2.969875    1.309970    2.838435
9.C      2.010745    0.664650    1.979857
10.N     1.409857    1.313495    0.941771
11.N     4.549954    1.139830    4.797249
12.O     0.789654   -1.284054    1.361309
13.C     4.271415   -0.890660   -3.897429
14.C     3.237762   -0.976303   -2.823462
15.C     2.336222   -0.066632   -2.319924
16.N     2.995539   -2.136439   -2.102367
17.C     1.993737   -1.896444   -1.214652

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21.C	-2.807097	-1.762954	-2.574869
22.C	-3.518142	-1.249418	-3.672321
23.C	-2.374046	2.303150	-3.666783
24.C	-1.881997	-0.980864	-1.857768
25.C	-3.392434	0.065663	-4.104355
26.C	-2.519290	0.923087	-3.383582
27.C	-1.753039	0.394785	-2.285449
28.N	-0.893921	1.172044	-1.563133
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31.Ni	0.039236	0.014218	-0.039553
32.C	-3.549225	1.892561	4.077658
33.C	-2.831389	1.142506	3.004874
34.C	-1.781773	1.471748	2.177268
35.N	-3.173047	-0.148092	2.630069
36.C	-2.347733	-0.544675	1.624896
37.N	-1.495006	0.420915	1.328199
38.H	-3.565574	0.928413	-5.952346
39.H	5.331708	1.546791	4.280578
40.H	4.151660	1.885909	5.369963
41.H	-2.981103	2.787696	4.353740
42.H	-4.550982	2.216638	3.755446
43.H	-3.671025	1.284460	4.986371
44.H	-3.906790	-0.712017	3.040877
45.H	-2.378103	-1.508135	1.133792
46.H	-1.213363	2.393423	2.153700
47.H	1.997614	-2.437500	3.413017
48.H	3.658199	-1.306046	4.881676
49.H	3.981776	3.204932	3.173614
50.H	2.881639	4.334600	1.237388
51.H	1.260325	3.058790	-0.148918
52.H	-0.119286	3.059263	-1.257207
53.H	-1.400845	4.139580	-3.090999
54.H	-2.971116	2.752330	-4.459387
55.H	-4.199790	-1.913065	-4.210139
56.H	-2.947632	-2.799467	-2.272773
57.H	5.234607	-1.308101	-3.568100
58.H	3.966793	-1.429609	-4.807801
59.H	4.441946	0.156503	-4.171081
60.H	2.188625	0.963858	-2.619489
61.H	1.610311	-2.615600	-0.503834
62.H	3.492001	-3.013268	-2.203625
63.H	-4.790559	-0.102266	-5.565606

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GEOMETRY

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BASIS

type TZ2P

core none

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END INPUT

Section S4. Results From DFT Calculations

S4.1. Optimized cartesian coordinates and molecular structure for *cis*-Quin BP86

1.C	2.243672	-2.200123	-2.447739
2.C	1.360933	-1.893156	-1.394585
3.C	2.799438	2.616302	-1.141645
4.C	3.698600	2.399606	-2.207384
5.C	3.067748	-1.211423	-2.947351
6.C	2.005525	1.580376	-0.626074
7.C	3.853038	1.168788	-2.829998
8.C	3.043509	0.087600	-2.381129
9.C	2.129828	0.305133	-1.300534
10.N	1.305921	-0.681032	-0.855962
11.N	4.730897	0.966737	-3.939152
12.O	1.184926	1.701304	0.390447
13.C	2.437509	-2.921593	4.885147
14.C	2.064950	-1.925891	3.831134
15.C	1.191833	-1.964906	2.765085
16.N	2.627534	-0.660128	3.769787
17.C	2.096791	0.004563	2.707069
18.N	1.223016	-0.765627	2.083426
19.C	-2.230928	2.201720	-2.454078
20.C	-1.351280	1.888106	-1.400375
21.C	-2.808029	-2.616503	-1.163603
22.C	-3.702722	-2.393864	-2.231841
23.C	-3.058864	1.218246	-2.957816
24.C	-2.014977	-1.583542	-0.640540
25.C	-3.852034	-1.160544	-2.850865
26.C	-3.039884	-0.083284	-2.396887
27.C	-2.130468	-0.307358	-1.314166
28.N	-1.303268	0.674198	-0.864963
29.N	-4.729238	-0.951703	-3.959357
30.O	-1.201994	-1.707004	0.382077
31.Ni	-0.013287	-0.005522	0.576671
32.C	-2.427966	2.938778	4.892530
33.C	-2.051687	1.931770	3.850598
34.C	-1.180547	1.961229	2.782162
35.N	-2.614942	0.665601	3.801692
36.C	-2.087768	-0.007876	2.742510
37.N	-1.214771	0.756352	2.110500
38.H	2.246748	-3.204075	-2.869882
39.H	0.667883	-2.626945	-0.986157
40.H	2.726432	3.605812	-0.691999
41.H	4.304043	3.239884	-2.555113
42.H	3.722499	-1.414158	-3.794235
43.H	5.203585	1.831942	-4.193106
44.H	5.443249	0.261482	-3.746542
45.H	3.191272	-2.508255	5.568697
46.H	1.569987	-3.213524	5.492666
47.H	2.859985	-3.835468	4.446808
48.H	0.543447	-2.769587	2.440290
49.H	3.318641	-0.290485	4.410766
50.H	2.346571	1.016193	2.412637

51.H	-2.229077	3.207099	-2.872524
52.H	-0.653711	2.616459	-0.990083
53.H	-2.740579	-3.607140	-0.715761
54.H	-4.311256	-3.230525	-2.582830
55.H	-3.712952	1.427587	-3.803558
56.H	-5.210097	-1.812993	-4.211642
57.H	-5.435512	-0.240471	-3.765605
58.H	-3.184399	2.533601	5.578505
59.H	-1.563133	3.239026	5.499372
60.H	-2.849143	3.847595	4.441786
61.H	-0.532818	2.762715	2.448374
62.H	-3.307134	0.302855	4.445567
63.H	-2.344242	-1.019720	2.454838

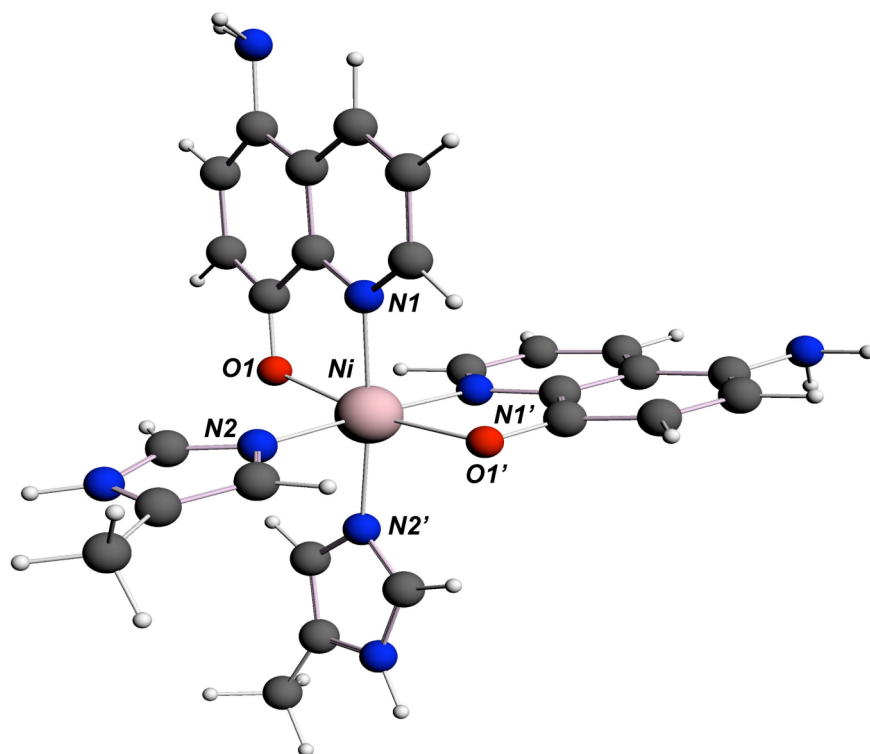


Figure S4.2. Optimized geometry of the model *cis*-Quin BP86

Bond (Å)	HQuin1	Model	% Difference
Ni-O1	2.1(1)	2.08	2.4
Ni-N1	2.1(1)	2.05	0.9
Ni-N2	2.0(1)	2.09	5.4
Ni-O1'	2.1(1)	2.09	2.4
Ni-N1'	2.1(1)	2.06	1.4
Ni-N2'	2.0(1)	2.09	4.4

Table S4.3. Calculated bond distances for the crystallographically determined HQuin1 and the computationally minimized *cis*-Quin BP86 model.

Angle (°)	HQuin1	Model	% Difference
O1-Ni-N1	82(1)	81.13	1.1
O1-Ni-N2	95(1)	92.17	3.0
O1-Ni-O1'	165(1)	169.50	2.7
O1-Ni-N1'	87(1)	91.84	5.4
O1-Ni-N2'	94(1)	96.16	2.3
N1-Ni-N2	91(1)	91.93	1.0
N1-Ni-O1'	87(1)	91.56	5.1
N1-Ni-N1'	91(1)	91.27	0.3
N1-Ni-N2'	175.1)	176.96	1.1
N2-Ni-O1'	95(1)	95.61	0.6
N2-Ni-N1'	176(1)	175.20	0.5
N2-Ni-N2'	86(1)	86.78	0.9

Table S4.4. Calculated bond angles for the crystallographically determined HQuin1 and the computationally minimized *cis*-Quin BP86 model.

S4.5. Optimized cartesian coordinates and molecular structure for *trans*-Quin BP86

1.C	2.660094	3.296980	1.484037
2.C	1.738059	2.579749	0.700783
3.C	2.257117	-1.394138	3.241701
4.C	3.190055	-0.752434	4.067420
5.C	3.266868	2.666845	2.550695
6.C	1.637437	-0.725907	2.166684
7.C	3.566179	0.574659	3.901047
8.C	2.969875	1.309970	2.838435
9.C	2.010745	0.664650	1.979857
10.N	1.409857	1.313495	0.941771
11.N	4.549954	1.139830	4.797249
12.O	0.789654	-1.284054	1.361309
13.C	4.271415	-0.890660	-3.897429
14.C	3.237762	-0.976303	-2.823462
15.C	2.336222	-0.066632	-2.319924
16.N	2.995539	-2.136439	-2.102367
17.C	1.993737	-1.896444	-1.214652
18.N	1.575301	-0.648081	-1.325296
19.C	-1.514654	3.071739	-2.910007
20.C	-0.789442	2.461934	-1.868925

21.C	-2.807097	-1.762954	-2.574869
22.C	-3.518142	-1.249418	-3.672321
23.C	-2.374046	2.303150	-3.666783
24.C	-1.881997	-0.980864	-1.857768
25.C	-3.392434	0.065663	-4.104355
26.C	-2.519290	0.923087	-3.383582
27.C	-1.753039	0.394785	-2.285449
28.N	-0.893921	1.172044	-1.563133
29.N	-4.157770	0.600180	-5.188135
30.O	-1.179946	-1.420262	-0.854001
31.Ni	0.039236	0.014218	-0.039553
32.C	-3.549225	1.892561	4.077658
33.C	-2.831389	1.142506	3.004874
34.C	-1.781773	1.471748	2.177268
35.N	-3.173047	-0.148092	2.630069
36.C	-2.347733	-0.544675	1.624896
37.N	-1.495006	0.420915	1.328199
38.H	-3.565574	0.928413	-5.952346
39.H	5.331708	1.546791	4.280578
40.H	4.151660	1.885909	5.369963
41.H	-2.981103	2.787696	4.353740
42.H	-4.550982	2.216638	3.755446
43.H	-3.671025	1.284460	4.986371
44.H	-3.906790	-0.712017	3.040877
45.H	-2.378103	-1.508135	1.133792
46.H	-1.213363	2.393423	2.153700
47.H	1.997614	-2.437500	3.413017
48.H	3.658199	-1.306046	4.881676
49.H	3.981776	3.204932	3.173614
50.H	2.881639	4.334600	1.237388
51.H	1.260325	3.058790	-0.148918
52.H	-0.119286	3.059263	-1.257207
53.H	-1.400845	4.139580	-3.090999
54.H	-2.971116	2.752330	-4.459387
55.H	-4.199790	-1.913065	-4.210139
56.H	-2.947632	-2.799467	-2.272773
57.H	5.234607	-1.308101	-3.568100
58.H	3.966793	-1.429609	-4.807801
59.H	4.441946	0.156503	-4.171081
60.H	2.188625	0.963858	-2.619489
61.H	1.610311	-2.615600	-0.503834
62.H	3.492001	-3.013268	-2.203625
63.H	-4.790559	-0.102266	-5.565606

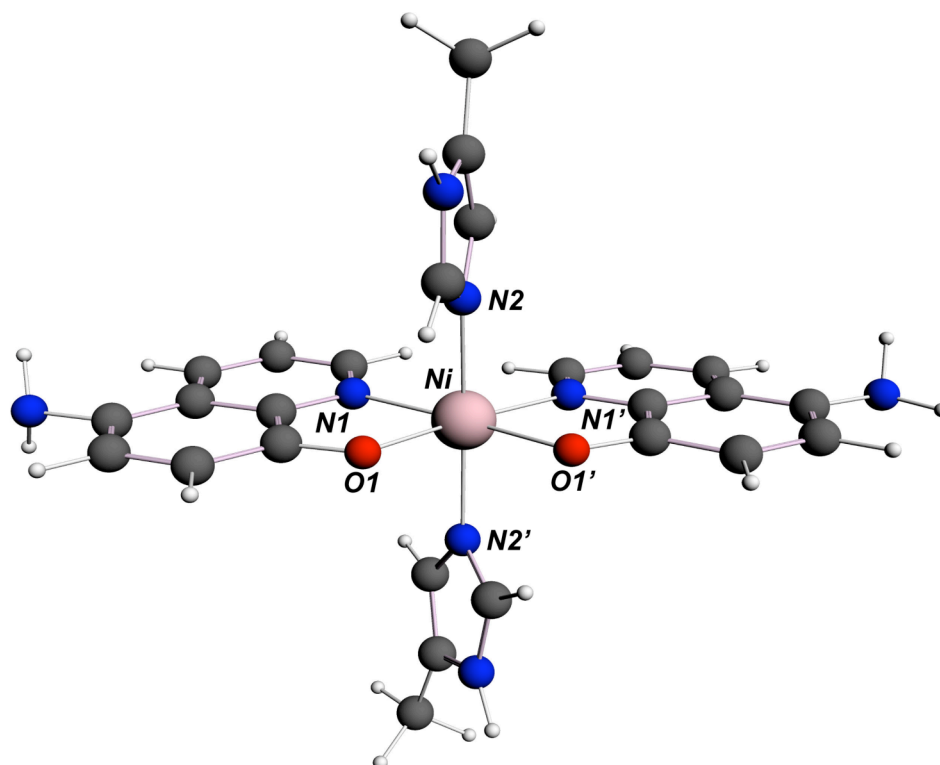


Figure S4.6. Optimized geometry of the model *trans*-Quin BP86

Bond (Å)	HQuin1	Model
Ni-O1	2.1(1)	2.05
Ni-N1	2.1(1)	2.12
Ni-N2	2.0(1)	2.11
Ni-O1'	2.1(1)	2.05
Ni-N1'	2.1(1)	2.13
Ni-N2'	2.0(1)	2.09

Table S4.7. Calculated bond distances for the crystallographically determined HQuin1 and the computationally minimized *trans*-Quin BP86 model.

Angle (°)	HQuin1	Model
O1-Ni-N1	82(1)	80.56
O1-Ni-N2	95(1)	87.23
O1-Ni-O1'	165(1)	92.23
O1-Ni-N1'	87(1)	173.16
O1-Ni-N2'	94(1)	86.84
N1-Ni-N2	91(1)	90.22
N1-Ni-O1'	87(1)	173.11
N1-Ni-N1'	91(1)	106.26
N1-Ni-N2'	175.1)	92.99
N2-Ni-O1'	95(1)	88.35
N2-Ni-N1'	176(1)	93.07
N2-Ni-N2'	86(1)	172.70

Table S4.8 Calculated bond angles for the crystallographically determined HQuin1 and the computationally minimized *trans*-Quin BP86 model.

S4.9 Optimized cartesian coordinates and molecular structure for *cis*-Quin OLYP

1.C	2.324995	-2.177402	-2.478191
2.C	1.430639	-1.872074	-1.437539
3.C	2.867517	2.624964	-1.150409
4.C	3.791858	2.412759	-2.186910
5.C	3.155835	-1.191411	-2.965747
6.C	2.059987	1.586694	-0.668409
7.C	3.955621	1.189069	-2.817221
8.C	3.129550	0.107263	-2.401356
9.C	2.193538	0.318493	-1.339842
10.N	1.363031	-0.663660	-0.903398
11.N	4.872934	1.005640	-3.896680
12.O	1.223783	1.702959	0.319531
13.C	2.462496	-2.955878	4.946702
14.C	2.090652	-1.962924	3.890640
15.C	1.209821	-1.996593	2.833081
16.N	2.658789	-0.705850	3.817510
17.C	2.125453	-0.047926	2.757788
18.N	1.240713	-0.804782	2.142232
19.C	-2.321022	2.180219	-2.489718
20.C	-1.433889	1.875469	-1.442589
21.C	-2.874521	-2.620583	-1.161013
22.C	-3.794273	-2.408355	-2.201797
23.C	-3.149440	1.194365	-2.981272

24.C	-2.067926	-1.583016	-0.675747
25.C	-3.953595	-1.184690	-2.834169
26.C	-3.127310	-0.103913	-2.415523
27.C	-2.197214	-0.315534	-1.349243
28.N	-1.369674	0.668074	-0.906764
29.N	-4.866099	-1.000228	-3.917340
30.O	-1.236685	-1.698894	0.316490
31.Ni	-0.004617	-0.001512	0.524658
32.C	-2.445798	2.957243	4.956962
33.C	-2.079467	1.959405	3.903715
34.C	-1.201231	1.986651	2.843713
35.N	-2.652612	0.704539	3.834681
36.C	-2.124593	0.041883	2.775329
37.N	-1.238583	0.794535	2.155126
38.H	2.332305	-3.178639	-2.899605
39.H	0.741942	-2.610262	-1.040697
40.H	2.784443	3.605460	-0.689020
41.H	4.410482	3.251841	-2.503542
42.H	3.818956	-1.404636	-3.798553
43.H	5.372840	1.866692	-4.083130
44.H	5.566984	0.294987	-3.684009
45.H	3.226210	-2.552520	5.619777
46.H	1.601225	-3.233789	5.563869
47.H	2.868103	-3.875094	4.511245
48.H	0.556797	-2.800288	2.525495
49.H	3.360096	-0.339139	4.441713
50.H	2.393184	0.956409	2.469082
51.H	-2.324857	3.181201	-2.911998
52.H	-0.748996	2.614604	-1.040664
53.H	-2.795039	-3.600683	-0.698206
54.H	-4.412888	-3.246735	-2.520232
55.H	-3.807176	1.407234	-3.818459
56.H	-5.373118	-1.858109	-4.099187
57.H	-5.554419	-0.282322	-3.710728
58.H	-3.206499	2.557413	5.635667
59.H	-1.581418	3.237663	5.568570
60.H	-2.853113	3.874582	4.519000
61.H	-0.545810	2.787195	2.532916
62.H	-3.354637	0.340952	4.460554
63.H	-2.398686	-0.961382	2.489082

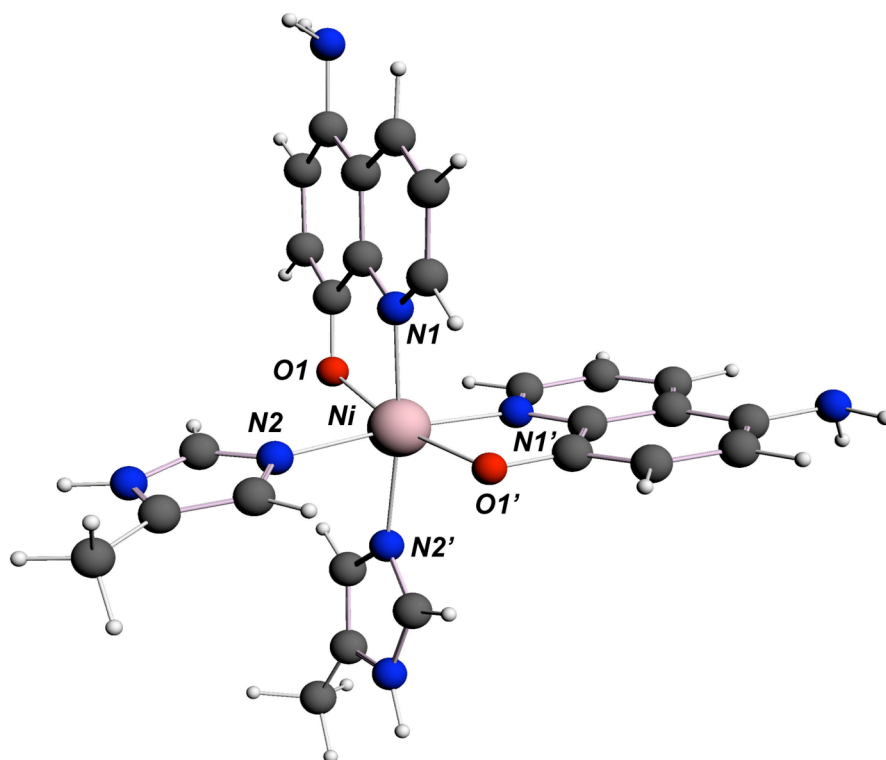


Figure S4.10. Optimized geometry of the model *cis*-Quin OLYP

Bond (Å)	HQuin1	Model	% Difference
Ni-O1	2.1(1)	2.11	0.5
Ni-N1	2.1(1)	2.09	0.5
Ni-N2	2.0(1)	2.19	9.1
Ni-O1'	2.1(1)	2.11	0.5
Ni-N1'	2.1(1)	2.09	0.5
Ni-N2'	2.0(1)	2.19	9.1

Table S4.11. Calculated bond distances for the crystallographically determined HQuin1 and the computationally minimized *cis*-Quin OLYP model.

Angle (°)	HQuin1	Model	% Difference
O1-Ni-N1	82(1)	78.94	3.8
O1-Ni-N2	95(1)	92.12	3.1
O1-Ni-O1'	165(1)	168.75	2.2
O1-Ni-N1'	87(1)	93.15	6.8
O1-Ni-N2'	94(1)	96.11	2.2
N1-Ni-N2	91(1)	90.94	0.1
N1-Ni-O1'	87(1)	93.44	7.1
N1-Ni-N1'	91(1)	93.5	2.7
N1-Ni-N2'	175.1	173.17	1.1
N2-Ni-O1'	95(1)	96.3	1.4
N2-Ni-N1'	176(1)	173.68	1.3
N2-Ni-N2'	86(1)	84.5	1.8

Table S4.12. Calculated bond angles for the crystallographically determined HQuin1 and the computationally minimized *cis*-Quin OLYP model.

S4.13 Optimized cartesian coordinates and molecular structure for *trans*-Quin OLYP

1.C	2.709784	3.303331	1.555393
2.C	1.790571	2.592947	0.767414
3.C	2.289799	-1.389086	3.281070
4.C	3.223172	-0.761191	4.110542
5.C	3.315579	2.668374	2.618011
6.C	1.678716	-0.704496	2.213458
7.C	3.608693	0.563278	3.958343
8.C	3.021263	1.312233	2.900064
9.C	2.062422	0.680296	2.033809
10.N	1.463331	1.328458	0.999943
11.N	4.587202	1.102247	4.871496
12.O	0.830521	-1.240239	1.410901
13.C	4.294914	-0.909563	-3.937319
14.C	3.263568	-0.999800	-2.864372
15.C	2.378459	-0.087877	-2.343424
16.N	3.004521	-2.162412	-2.163782
17.C	2.012228	-1.919896	-1.273139
18.N	1.611231	-0.667479	-1.358327
19.C	-1.570287	3.069186	-2.976251
20.C	-0.839189	2.467589	-1.937393
21.C	-2.818447	-1.768362	-2.624541
22.C	-3.536654	-1.269305	-3.718110
23.C	-2.427927	2.296483	-3.727214
24.C	-1.905327	-0.968248	-1.915853
25.C	-3.432751	0.043553	-4.157461

26.C	-2.568771	0.917531	-3.444059
27.C	-1.794019	0.404310	-2.346175
28.N	-0.940040	1.182888	-1.626097
29.N	-4.215082	0.547238	-5.244270
30.O	-1.200132	-1.389471	-0.920679
31.Ni	0.042965	0.025821	-0.044044
32.C	-3.577651	1.901728	4.131046
33.C	-2.870658	1.154878	3.051283
34.C	-1.834423	1.483623	2.211020
35.N	-3.203905	-0.135919	2.689531
36.C	-2.386046	-0.529861	1.684238
37.N	-1.542476	0.433380	1.369310
38.H	-3.630346	0.859583	-6.014688
39.H	5.383105	1.488017	4.370400
40.H	4.198257	1.862513	5.423793
41.H	-3.031844	2.815987	4.373913
42.H	-4.595760	2.188228	3.836772
43.H	-3.652415	1.309093	5.051278
44.H	-3.930100	-0.700429	3.101667
45.H	-2.427233	-1.499834	1.217143
46.H	-1.276069	2.406935	2.180955
47.H	2.022083	-2.429217	3.443630
48.H	3.682086	-1.324430	4.919682
49.H	4.024580	3.209322	3.238817
50.H	2.930447	4.340400	1.317614
51.H	1.312634	3.078691	-0.074194
52.H	-0.164718	3.067158	-1.338256
53.H	-1.459210	4.133912	-3.161808
54.H	-3.020935	2.747034	-4.517321
55.H	-4.209090	-1.945495	-4.246181
56.H	-2.944182	-2.803002	-2.318431
57.H	5.272032	-1.272730	-3.595223
58.H	4.016743	-1.490338	-4.826308
59.H	4.420960	0.130406	-4.247176
60.H	2.248942	0.945377	-2.629865
61.H	1.625514	-2.655558	-0.587134
62.H	3.482396	-3.042830	-2.276701
63.H	-4.818021	-0.181765	-5.607609

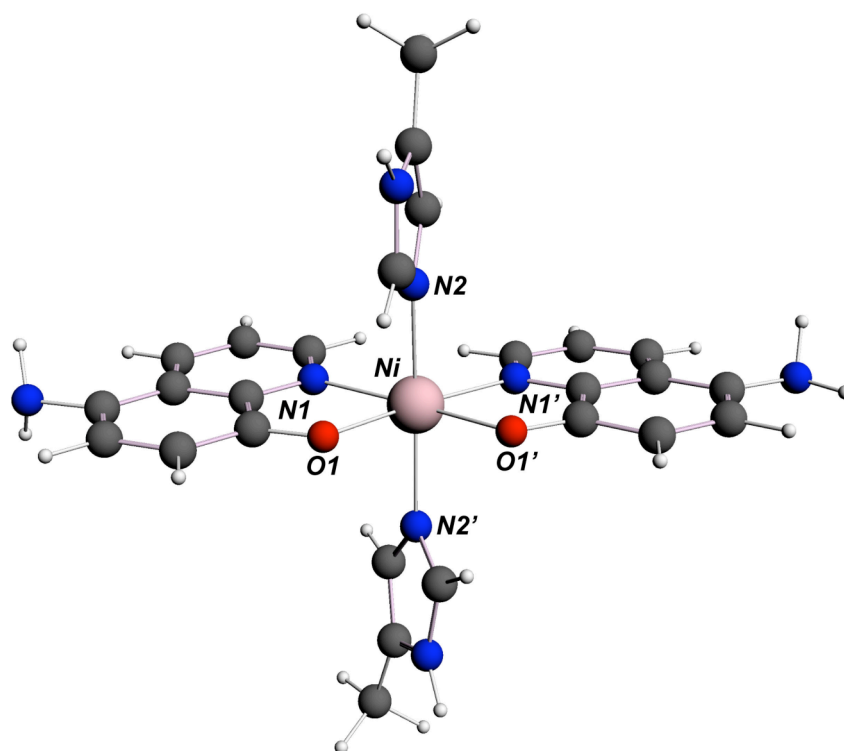


Figure S4.14. Optimized geometry of the model *trans*-Quin OLYP

Bond (Å)	HQuin1	Model
Ni-O1	2.1(1)	2.07
Ni-N1	2.1(1)	2.19
Ni-N2	2.0(1)	2.16
Ni-O1'	2.1(1)	2.08
Ni-N1'	2.1(1)	2.19
Ni-N2'	2.0(1)	2.16

Table S4.15. Calculated bond distances for the crystallographically determined HQuin1 and the computationally minimized *trans*-Quin OLYP model.

Angle (°)	HQuin1	Model
O1-Ni-N1	82(1)	77.69
O1-Ni-N2	95(1)	87.65
O1-Ni-O1'	165(1)	96.14
O1-Ni-N1'	87(1)	173.46
O1-Ni-N2'	94(1)	88.02
N1-Ni-N2	91(1)	93.2
N1-Ni-O1'	87(1)	173.11
N1-Ni-N1'	91(1)	108.69
N1-Ni-N2'	175.1)	92.49
N2-Ni-O1'	95(1)	87.44
N2-Ni-N1'	176(1)	90.87
N2-Ni-N2'	86(1)	171.96

Table S4.16. Calculated bond angles for the crystallographically determined HQuin1 and the computationally minimized *trans*-Quin OLYP model.