Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Material

G-quadruplex DNA binding properties of novel nickel Schiff base complexes with four pendant groups

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Table S1: Crystal data and structure refinement for **(5)** and **(9)**.

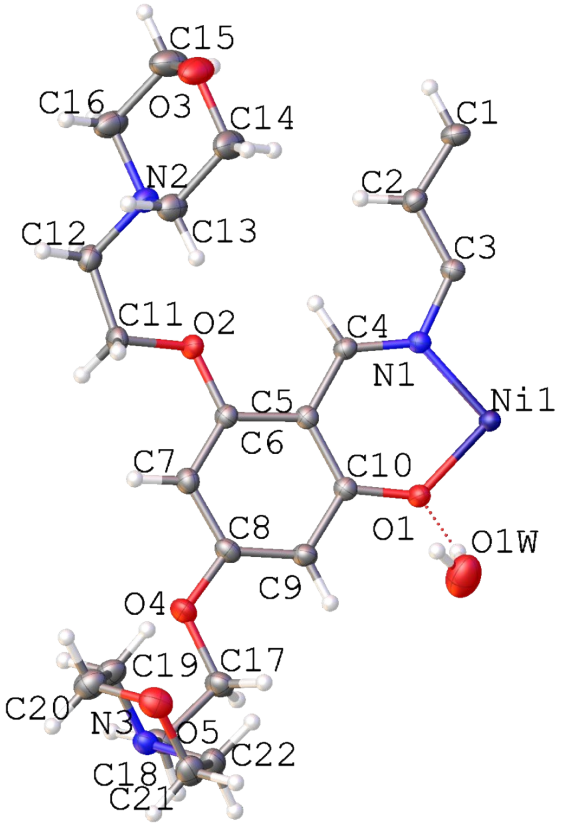
Identification code	**(5)**	**(9)**
Empirical formula	$C_{48.5}ClH_{69}N_6NiO_7$	$C_{44}H_{62}N_6NiO_{12}$
Formula weight	942.25	925.70
Temperature/K	150.00(10)	150.00(10)
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	*C*2/c
a/Å	11.7197(8)	30.6127(5)
b/Å	12.5847(8)	15.8401(3)
c/Å	16.6523(10)	9.8494(2)
α/°	101.829(6)	90
β/°	96.030(5)	96.209(2)
γ/°	97.639(6)	90
Volume/Å^3	2360.3(3)	4748.04(15)
Z	2	4
ρ_{calc}g/cm^3	1.326	1.295
μ/mm^{-1}	0.525	0.474
F(000)	1006.0	1968.0
Crystal size/mm^3	0.51 × 0.22 × 0.03	0.34 × 0.21 × 0.06
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.718 to 57.396	4.768 to 59.15
Index ranges	$-15 \le h \le 15$, $-17 \le k \le 16$, $-22 \le l \le 22$	$-42 \le h \le 42$, $-22 \le k \le 21$, $-13 \le l \le 13$
Reflections collected	55431	64511
Independent reflections	11983 [R_{int} = 0.0589, R_{sigma} = 0.0567]	6653 [R_{int} = 0.0328, R_{sigma} = 0.0214]
Data/restraints/parameters	11983/0/560	6653/0/288
Goodness-of-fit on F^2	1.058	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0437, wR_2 = 0.0990	R_1 = 0.0348, wR_2 = 0.0989
Final R indexes [all data]	R_1 = 0.0681, wR_2 = 0.1076	R_1 = 0.0432, wR_2 = 0.1028
Largest diff. peak/hole / e Å^{-3}	0.42/-0.71	0.52/-0.65
CCDC	2271794	2271795

Table S2: Binding free energies obtained from docking studies performed using nickel Schiff base complexes and either 1KF1 or 1KBD.

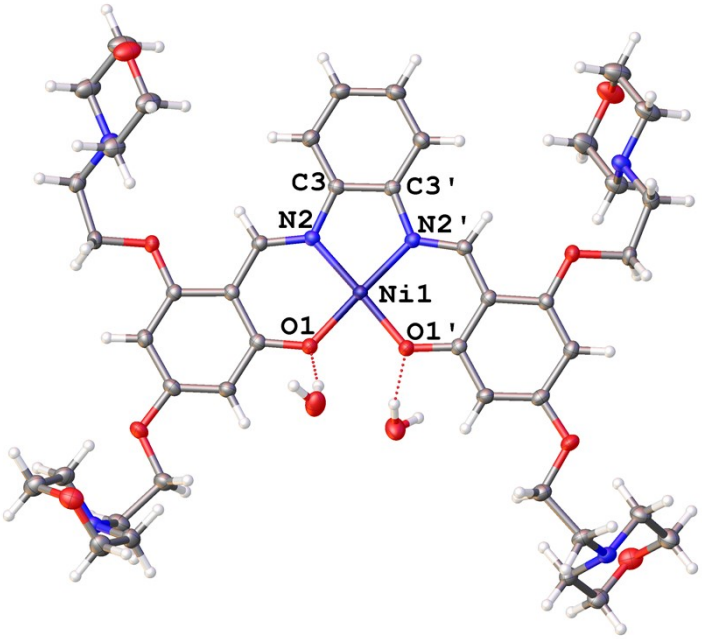
Complex	1KF1(qDNA)		1KBD (dsDNA)	
	ΔG (kcal/mol)[a]	Binding mode[b]	ΔG (kcal/mol)[a]	Binding mode[b]
(5)	-9.64 ± 0.05	Top, end stacking	-8.8 ± 0.10	Minor groove
(9)	-9.86 ± 0.05	Top, end stacking	-8.78 ± 0.08	Minor groove
(10)	-9.42 ± 0.04	Top, end stacking	-8.3 ± 0.20	Minor groove

[a] Average values of ΔG with standard errors obtained from the top five docking scores.

[b] "Top" or "Bottom" indicates which terminal G-tetrad was the preferred binding site.



(a)



(b)

Figure S1: (a) Additional illustrations of the molecular structure of **(9)**. (a) Asymmetric unit with displacement ellipsoids set to 50%. (b) Complex together with locations of both partial water molecules.

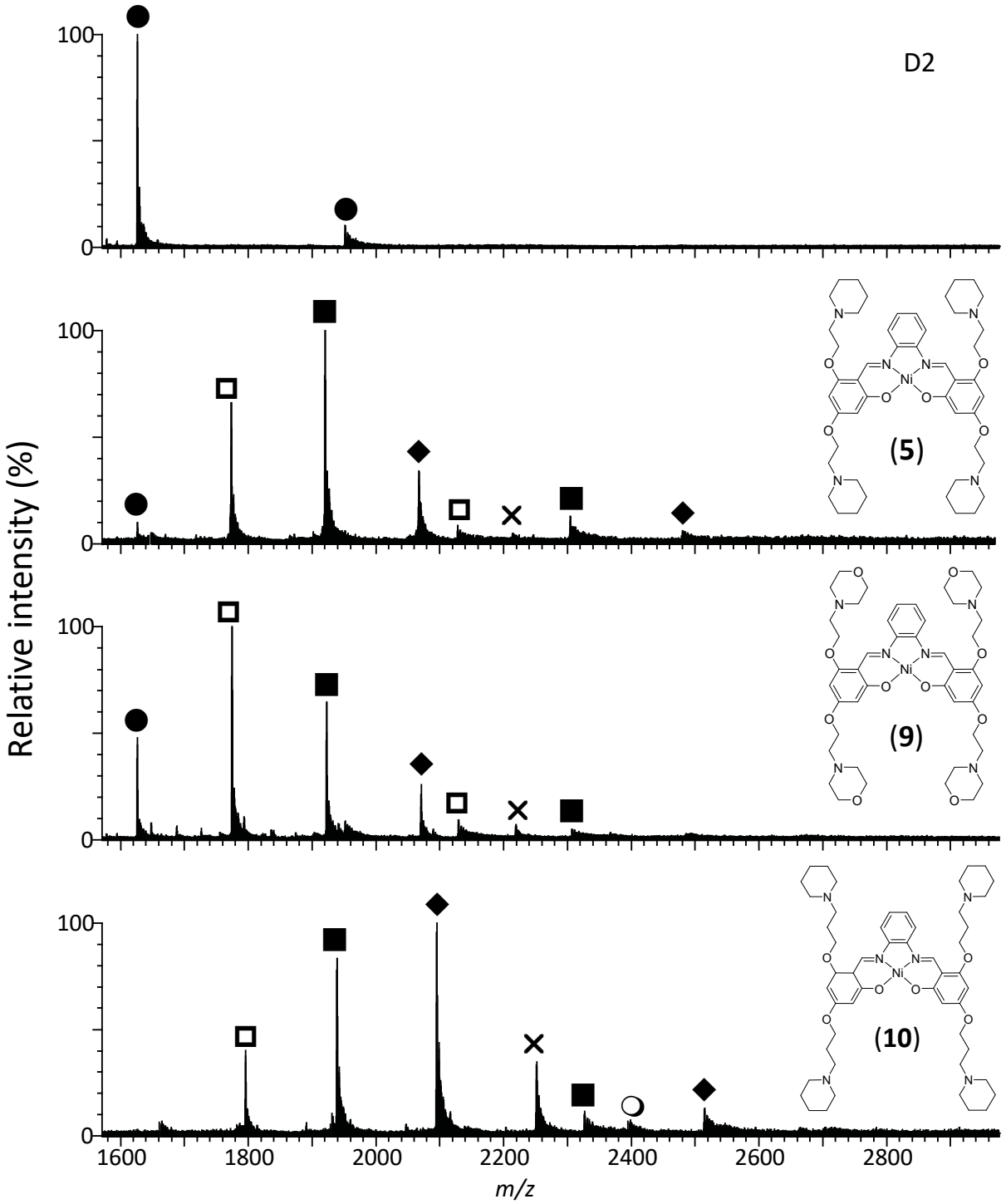


Figure S2: Negative ion ESI mass spectra of solutions containing different nickel Schiff base complexes and D2 at a 6:1 ratio. ● = Free D2; □ = [D2 + 1(Ni)]; ■ = [D2 + 2(Ni)]; ◆ = [D2 + 3(Ni)]; ✕ = [D2 + 4(Ni)]; ❍= [D2 + 5(Ni)].

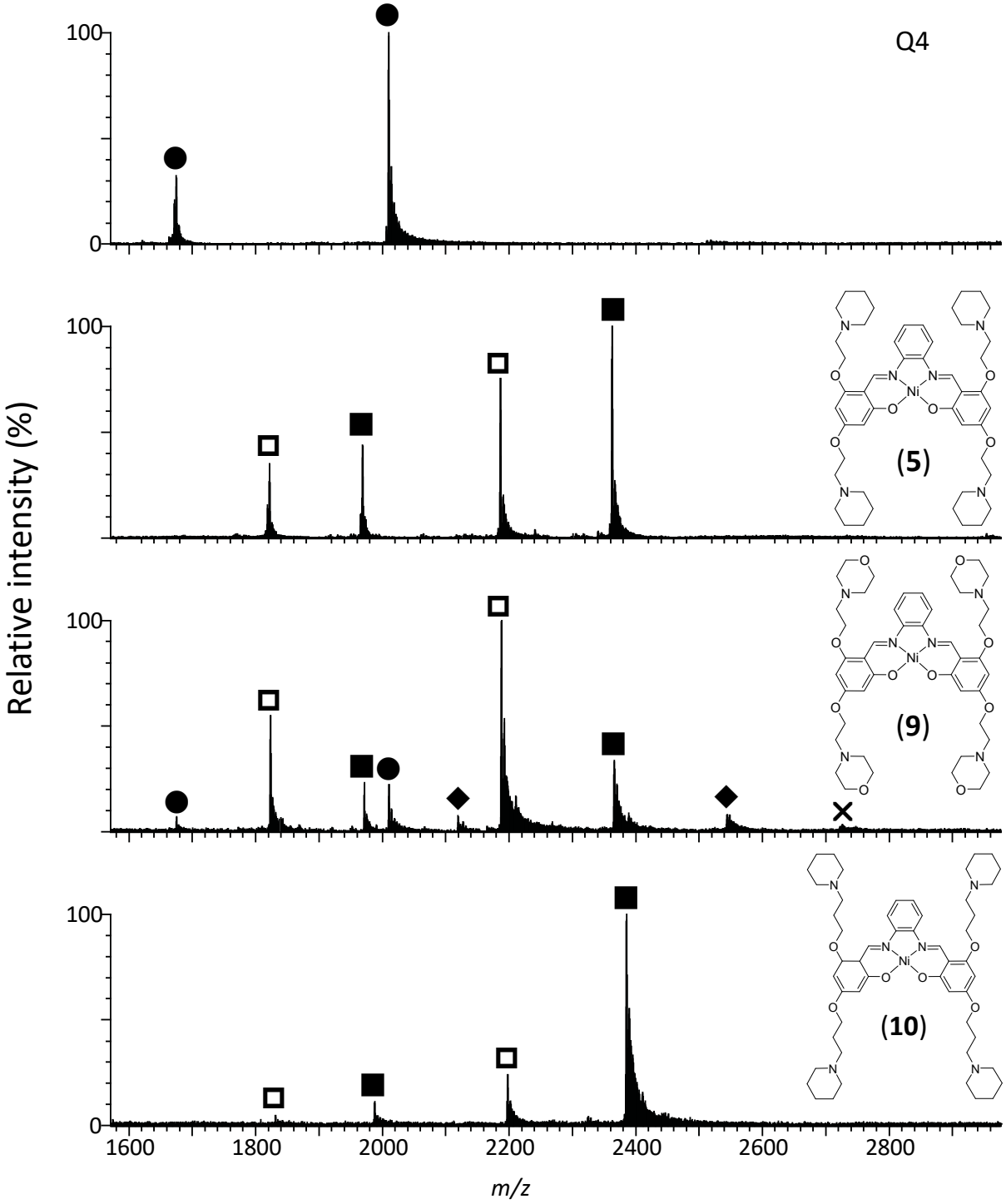


Figure S3: Negative ion ESI mass spectra of solutions containing different nickel Schiff base complexes and Q4 at a 6:1 ratio. ● = Free Q4; ☐ = [Q4 + 1(Ni)]; ■ = [Q4 + 2(Ni)]; ◆ = [Q4 + 3(Ni)]; ✕ = [Q4 + 4(Ni)]; ❍= [Q4 + 5(Ni)].

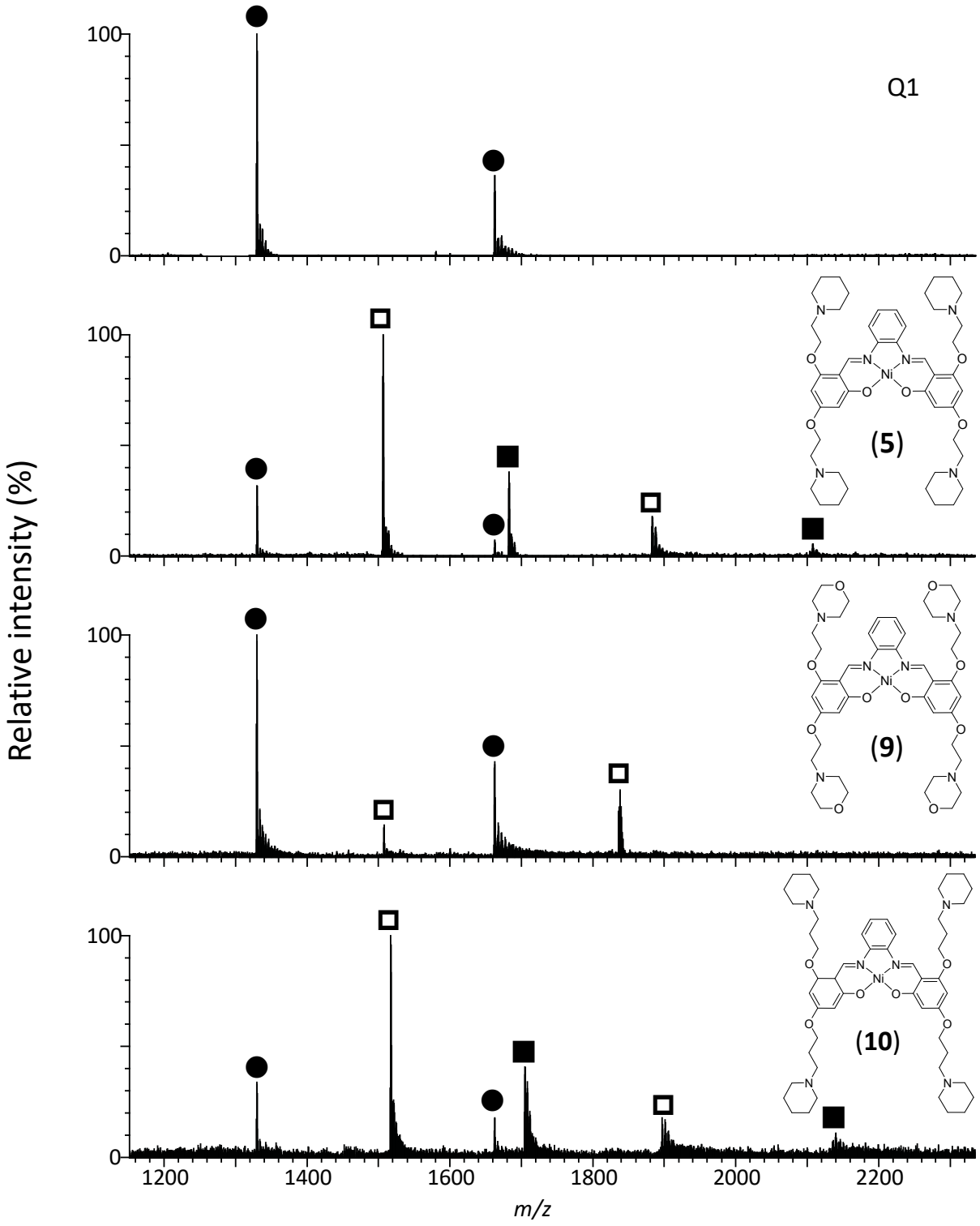


Figure S4: Negative ion ESI mass spectra of solutions containing different nickel Schiff base complexes and Q1 at a 6:1 ratio. ● = Free Q1; ☐ = [Q1 + 1(Ni)]; ■ = [Q1 + 2(Ni)]; ◆ = [Q1 + 3(Ni)]; ✕ = [Q1 + 4(Ni)]; ❍= [Q1 + 5(Ni)].

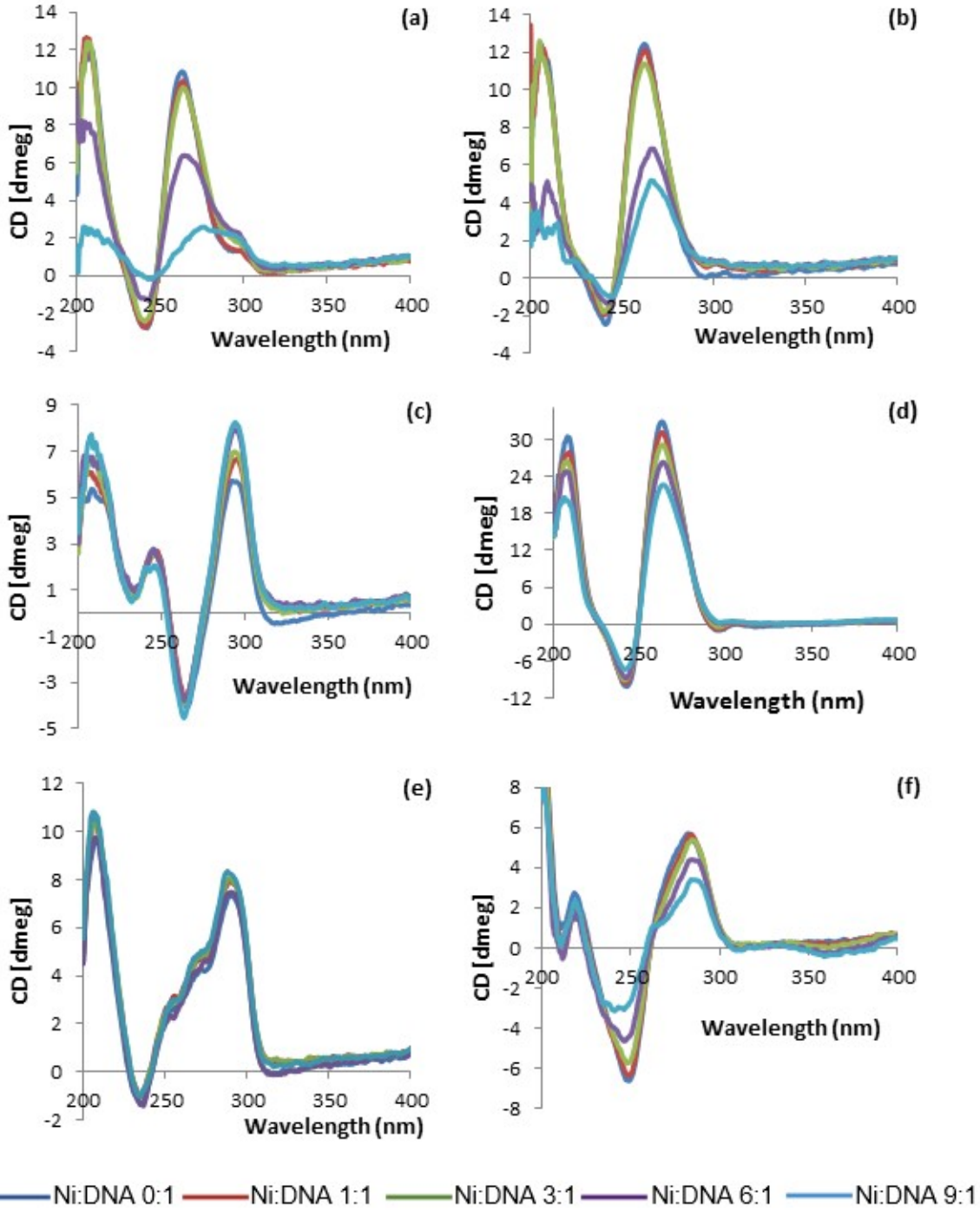


Figure S5: Circular dichroism spectra of solutions containing varying ratios of (**9**) and different DNA molecules: (a) Parallel Q1; (b) Parallel c-kit1; (c) Anti-parallel Q1; (d) Parallel Q4; (e) Hybrid Q1 and (f) D2.

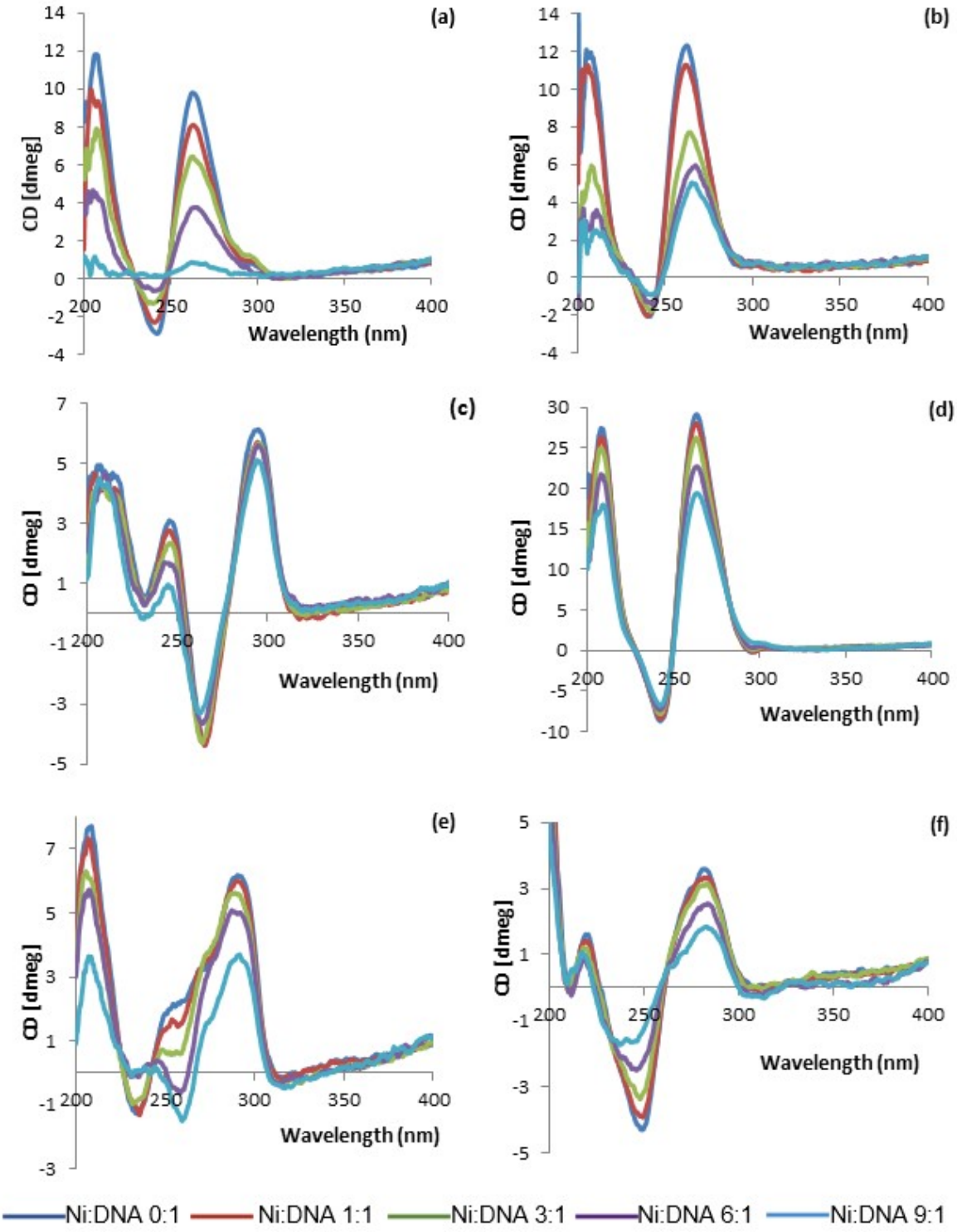


Figure S6: Circular dichroism spectra of solutions containing varying ratios of **(5)** and different DNA molecules: (a) Parallel Q1; (b) Parallel c-kit1; (c) Anti-parallel Q1; (d) Parallel Q4; (e) Hybrid Q1 and (f) D2.

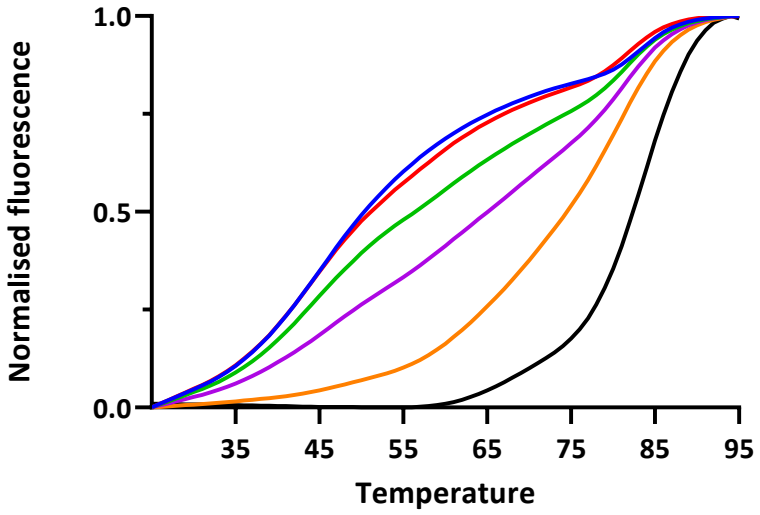


Figure S7: Results obtained from FRET melting assays performed using anti-parallel F21T and increasing concentrations of **(5)**.

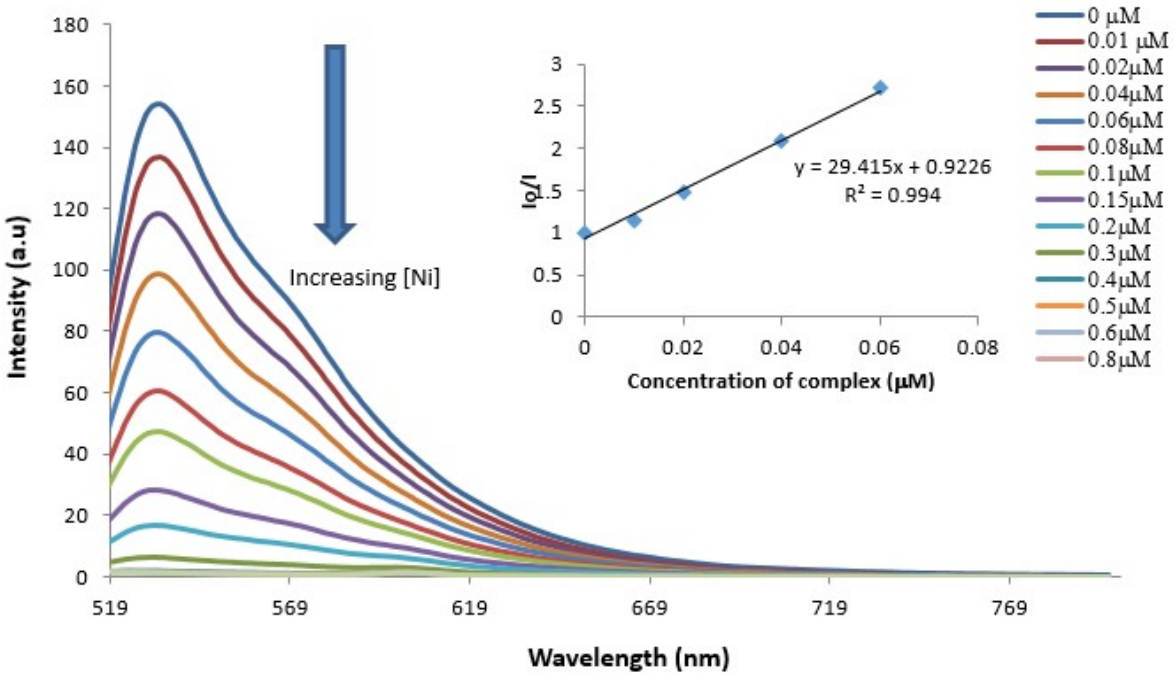


Figure S8: Results from an FID assay performed by adding increasing amounts of (**10**) to a solution containing thiazole orange and parallel Q4. The inset shows a Stern-Volmer plot derived from the data, which was then used to determine the DC_{50} for the nickel complex.