Multi-factors (Tail/Loop/Link/Ions) Regulation for G-quadruplexes Enantioselectivity of Δ- and Λ- $[Ru(bpy)_2(dppz\text{-}idzo)]^{2+}$

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Supplementary

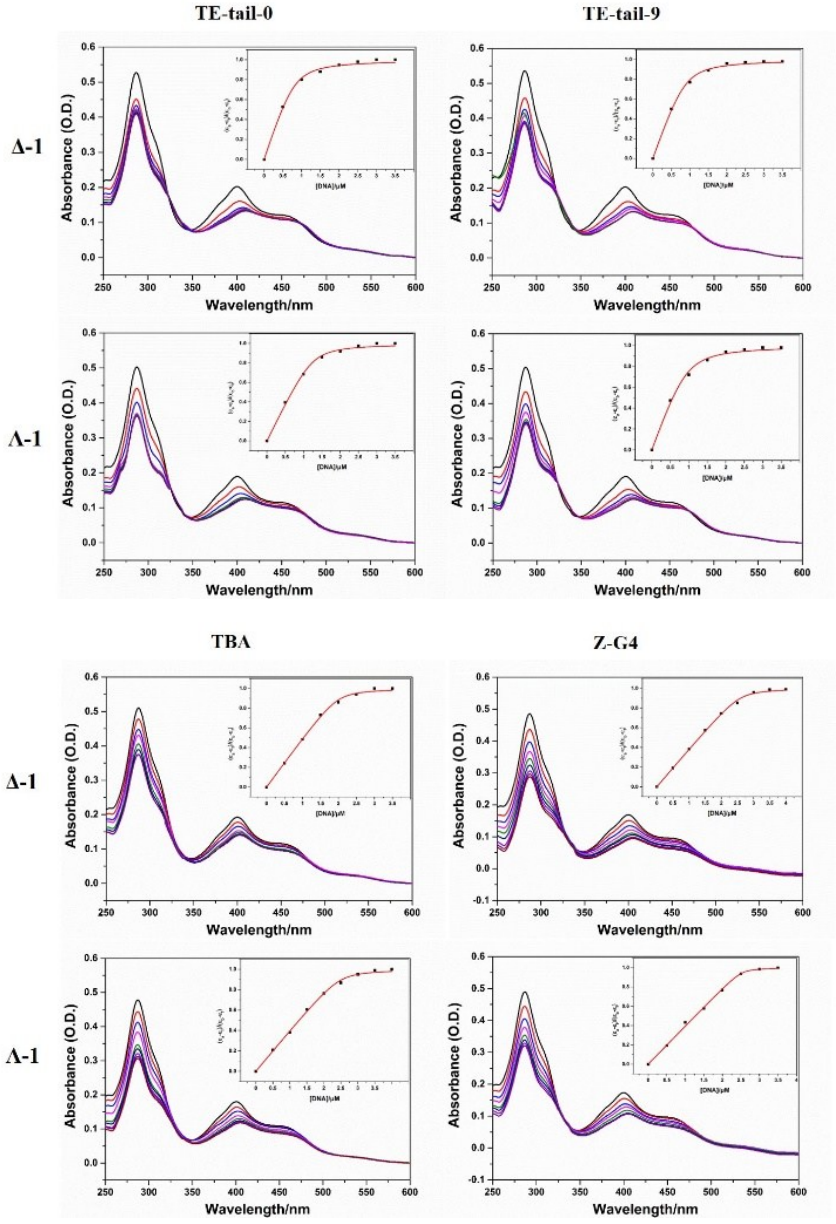


Figure S1. Absorption spectra of two isomers (8 μM) titrated by GQs.

Table S1. Binding constants and absorption spectra of **Δ/Λ**-1 for different GQs.

		TE-tail-0	TE-tail-9	TBA	Z-G4
K_b (10^6)	**Δ-1**	3.25	3.03	1.45	4.88
	Λ-1	3.61	2.92	1.91	5.62
$\lambda_{max\ /free}$	**Δ-1**	400	400	400	400
	Λ-1	400	400	400	400
$\lambda_{max\ /bound}$	**Δ-1**	406	409	403	402
	Λ-1	411	409	409	408
Δλ	**Δ-1**	6	9	3	2
	Λ-1	11	9	9	8
H(%)	**Δ-1**	28.8	38.9	29.0	38.4
	Λ-1	33.6	38.7	36.1	46.2

Δλ : Red shift.
H(%): Hypochromism for the absorbance at 400 nm.

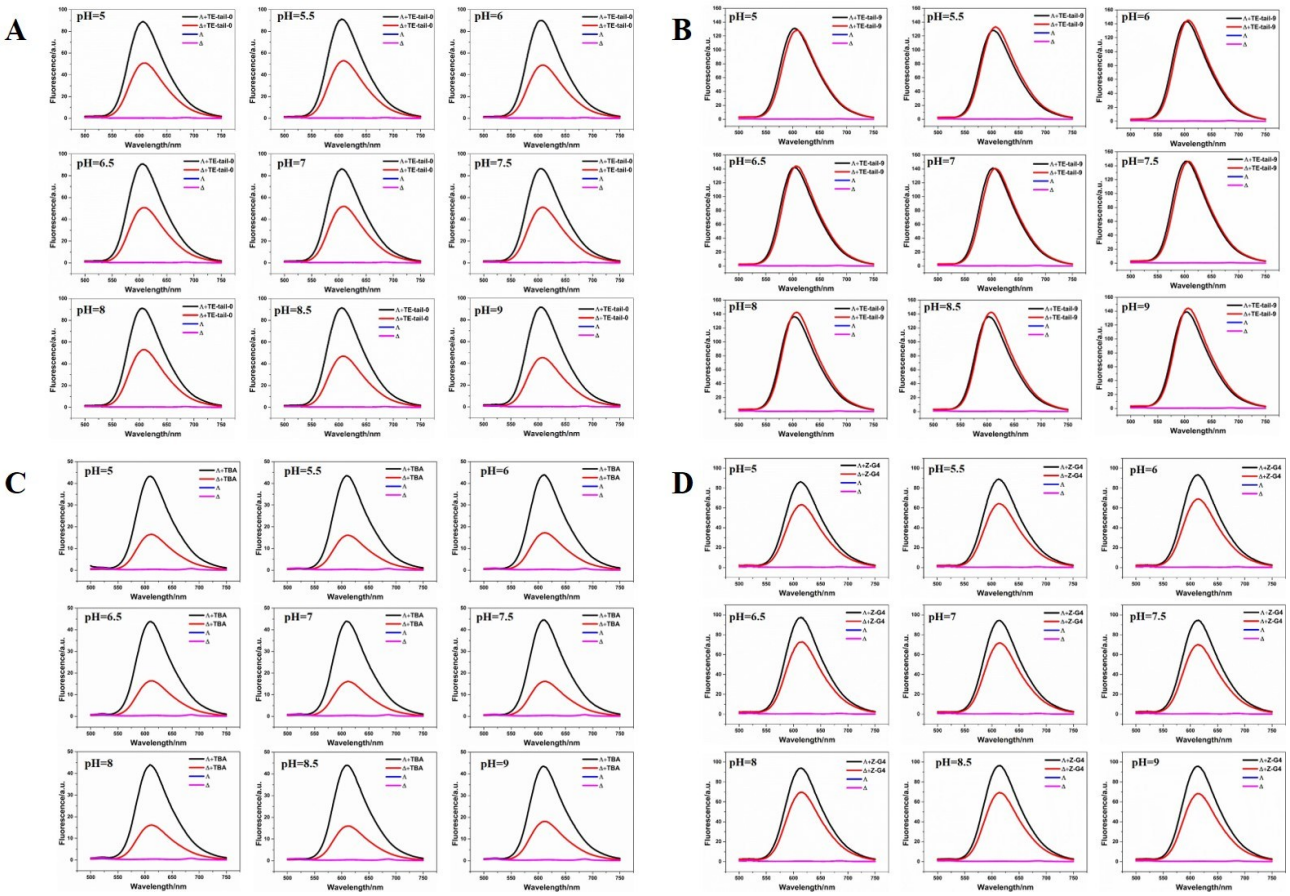


Figure S2. Comparison of emission observed for 1 μM enantiomers in the system of A) **TE-tail-0,** B) **TE-tail-9**, C) **TBA** and D) **Z-G4** with different pH in 10 mM Tris-HCl, 100 mM KCl buffer.

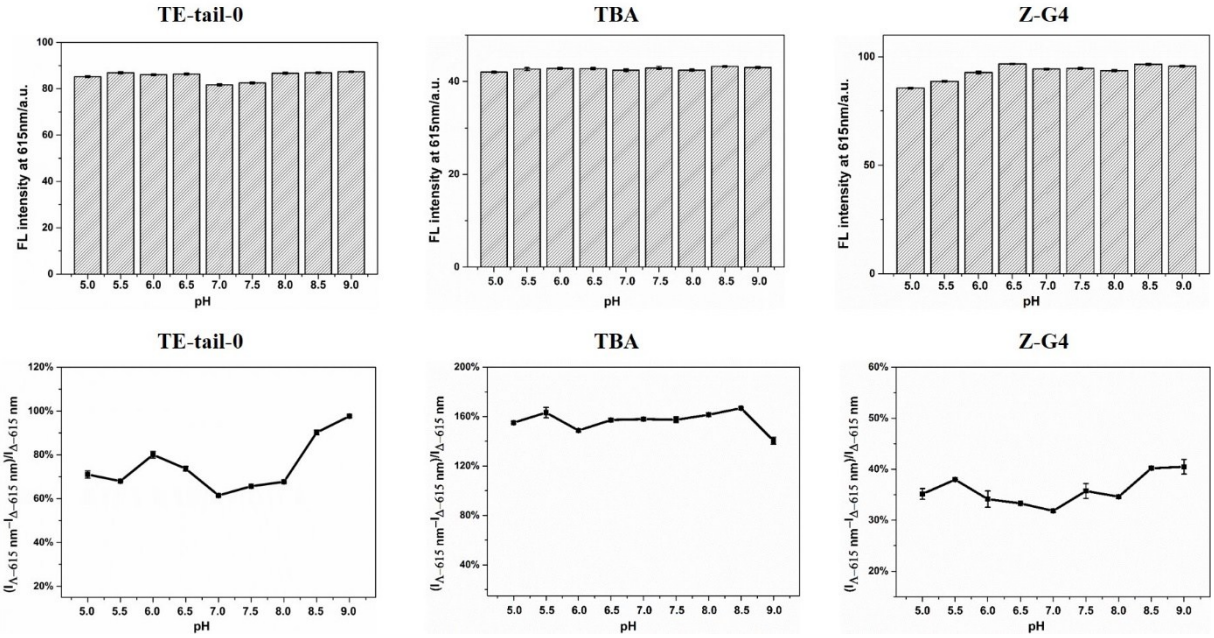


Figure S3. (Above) Comparison of emission in 615 nm observed for 1 μM enantiomers of **Λ-1** in the presence of 0.5 μM GQs with different pH; (Below) the enantioselectivity of **Δ/Λ-1** for GQs with different pH.

Table S2. Optimized structure of $[Ru(bpy)_2(dppz\text{-}idzo)]^{2+}$ in gas at the B3LYP//SDD/6-311G** level. E=-2219.252033 Hartree.

N	-3.71499800	1.14484500	-0.93687500	H	-6.47061600	-3.43586800	2.40266700
C	-4.02282500	2.32449000	-0.32964300	N	-2.34370700	-1.68139400	-1.25748300
C	-4.38685700	0.79563600	-2.04977300	C	-3.24246800	-2.63374100	-0.88357400
C	-5.01342200	3.16148100	-0.84635900	C	-1.59481500	-1.89362700	-2.35558300
C	-5.37945700	1.58609600	-2.60969400	C	-3.39090600	-3.81016800	-1.62014300
H	-4.10732400	-0.14859700	-2.49651600	C	-1.69926300	-3.04120500	-3.12765900
C	-5.69994100	2.79306200	-1.99570200	H	-0.89562700	-1.10973300	-2.61260400
H	-5.25244300	4.09448900	-0.35549600	C	-2.61462200	-4.01972700	-2.75231400
H	-5.88690800	1.25560700	-3.50671700	H	-4.10480600	-4.56152600	-1.31314100
H	-6.47060700	3.43588000	-2.40266600	H	-1.07164300	-3.15913500	-4.00146500
N	-2.34370400	1.68139600	1.25748500	H	-2.72263100	-4.93002700	-3.32888700
C	-1.59481200	1.89362700	2.35558500	C	0.53956900	2.40878100	-2.47921300
C	-3.24246500	2.63374400	0.88357800	C	1.77734200	1.98352500	-2.03447800
C	-1.69926000	3.04120300	3.12766400	C	1.84315000	1.00509900	-1.02930800
H	-0.89562400	1.10973200	2.61260500	C	0.63324300	0.50287100	-0.51799000
C	-3.39090300	3.81016900	1.62015000	C	-0.61862800	1.85877300	-1.92427900
C	-2.61461900	4.01972600	2.75232100	C	0.63324300	-0.50287800	0.51798300
H	-1.07163900	3.15913200	4.00147000	C	1.84315000	-1.00511100	1.02929600
H	-4.10480300	4.56152700	1.31315000	C	1.77734200	-1.98353500	2.03446800
H	-2.72262800	4.93002500	3.32889600	H	2.70008700	-2.38068400	2.43702100
N	-3.71499900	-1.14484100	0.93687800	C	0.53956900	-2.40878600	2.47920800
C	-4.02282900	-2.32448500	0.32964700	C	-0.61862800	-1.85877300	1.92427900
C	-4.38685700	-0.79563000	2.04977600	H	0.45058400	3.16157900	-3.25201200
C	-5.01342800	-3.16147300	0.84636100	H	2.70008700	2.38067100	-2.43703400
C	-5.37946000	-1.58608700	2.60969700	H	-1.59873300	2.17238100	-2.25818200
H	-4.10732200	0.14860200	2.49652000	H	0.45058400	-3.16158300	3.25200900
C	-5.69994700	-2.79305200	1.99570400	H	-1.59873300	-2.17237700	2.25818600
H	-5.25245200	-4.09448000	0.35549800	N	-0.58414300	-0.92451600	0.96683300
H	-5.88691000	-1.25559700	3.50672000	N	-0.58414300	0.92451400	-0.96683500

C	3.10804700	0.49847100	-0.50818600	C	7.78637000	0.50796900	-0.51637900
C	3.10804700	-0.49848800	0.50817000	C	7.78637000	-0.50799300	0.51635600
N	4.24160000	0.98563800	-1.00421400	C	9.96856000	-0.00010300	-0.00010100
N	4.24160000	-0.98566100	1.00419200	N	9.10202900	-0.77676800	0.78953700
C	5.39882000	0.51066800	-0.51972100	H	9.45891200	-1.43840300	1.46193500
C	6.62379100	1.01349000	-1.03062100	Ru	-2.22062200	0.00000100	0.00000100
C	5.39882000	-0.51070300	0.51968700	O	11.16491200	0.00005300	0.00005200
H	6.60126400	1.77182300	-1.80184300	N	9.10202900	0.77682200	-0.78948300
C	6.62379100	-1.01348700	1.03062400	H	9.45891200	1.43861800	-1.46172400
H	6.60126400	-1.77178200	1.80188400				

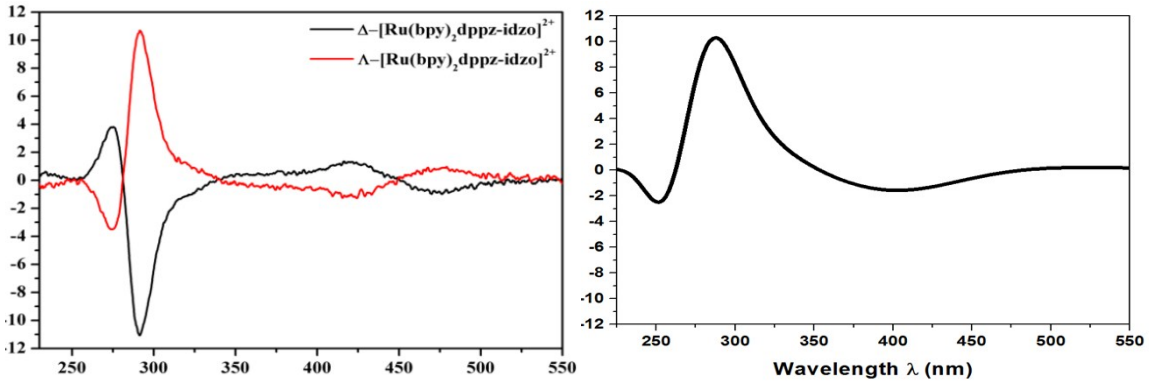


Figure S4. A) CD spectra of 4 μM **Δ-1** and **Λ-1** in the buffer of Tris-KCl; B) Calculated CD spectra of the **Λ-1**.

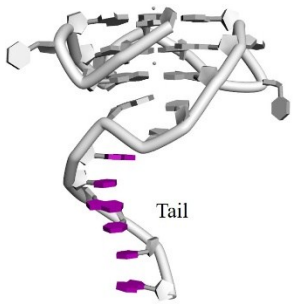


Figure S5. Schematic representation of **TE-tail-9** with a single-strand DNA in the 3'-end.

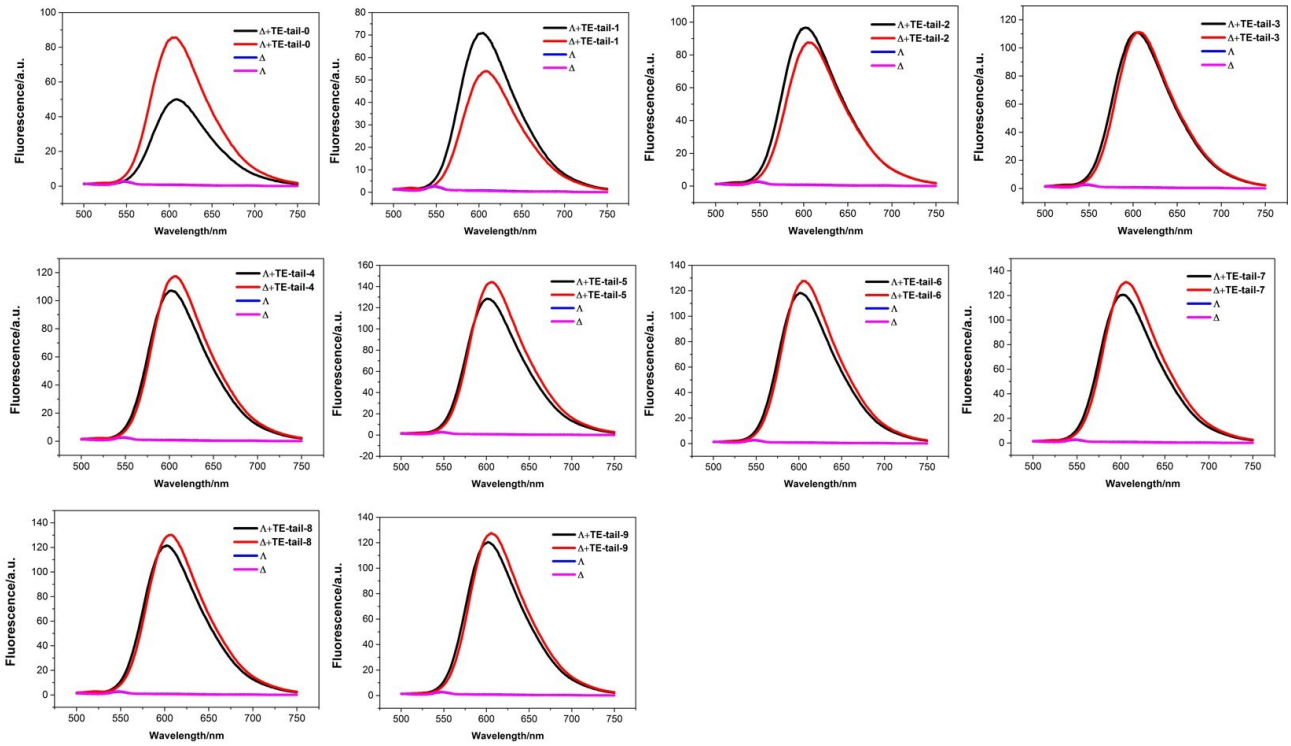


Figure S6. Comparison of emission observed for 1 μM enantiomers in the 0.5 μM **TE-tail-n** with different tail-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

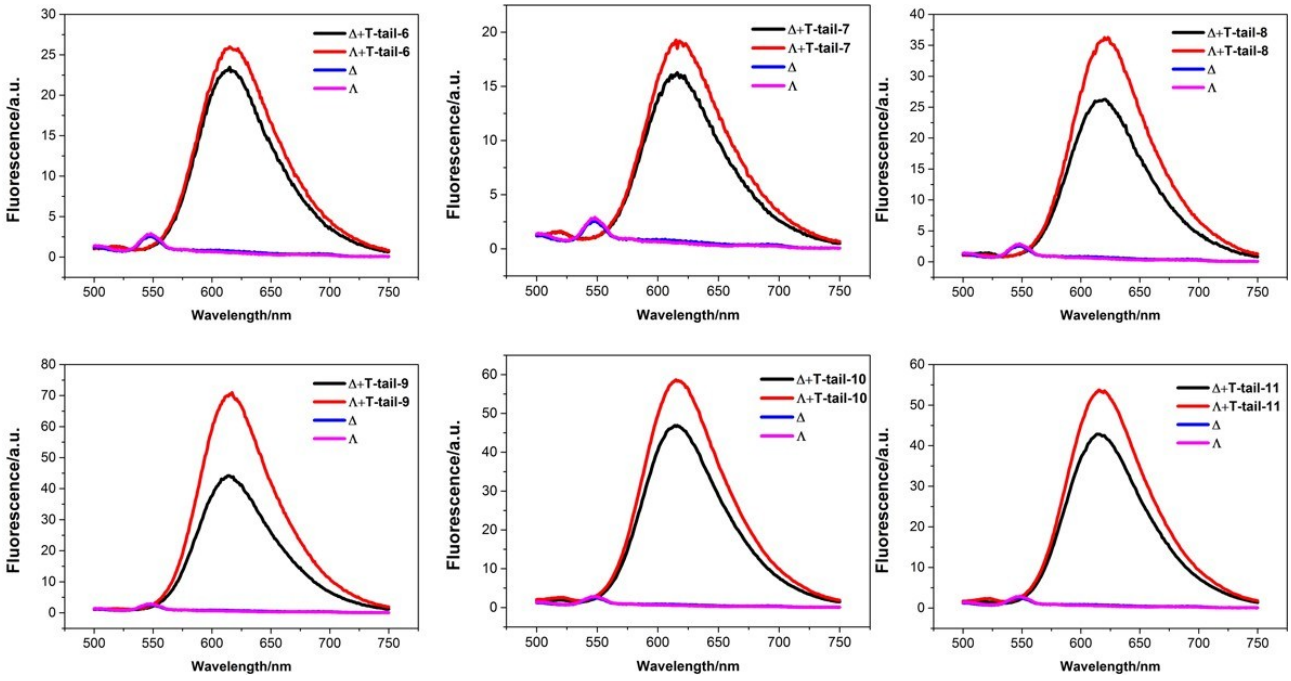


Figure S7. Comparison of emission observed for 1μM enantiomers in the 0.5 μM **T-tail-n** with different tail-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

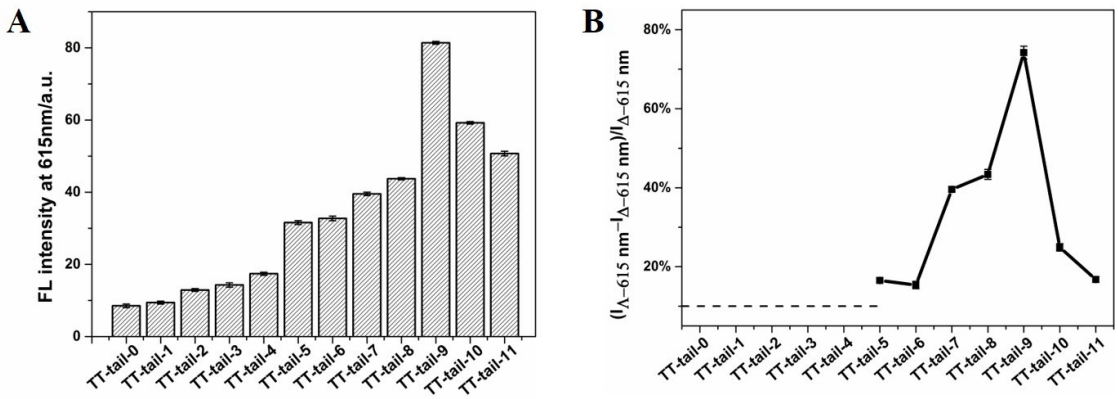


Figure S8. A) Comparison of emission in 615 nm observed for 1 μM enantiomers of **Λ-1** in the presence of 0.5 μM **TT-tail-n**; B) the enantioselectivity of chiral Ru-complex for **TT-tail-n**.

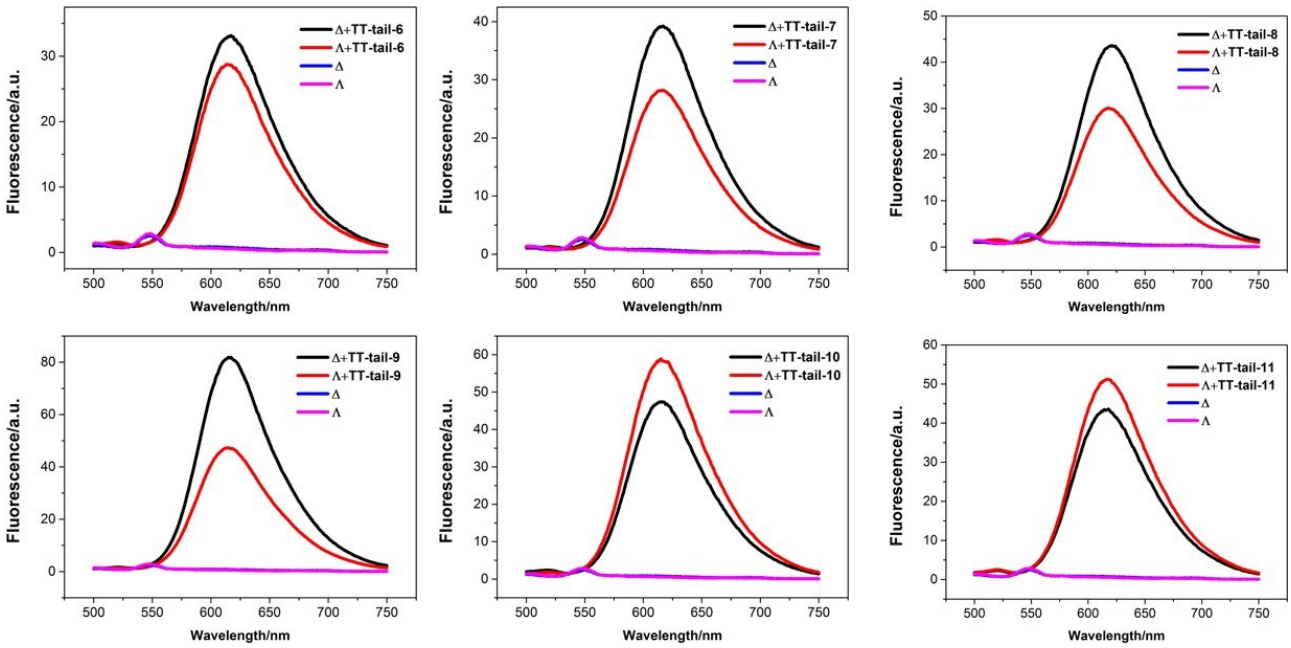


Figure S9. Comparison of emission in 615 nm observed for 1 μM enantiomers in the presence of 0.5 μM **TT-tail-n** with different tail-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH 7.4.

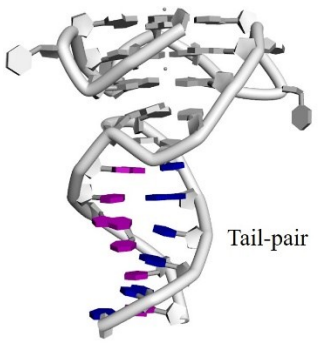


Figure S10. Schematic representation of **T-tail-pair** with a B-form duplex DNA tail.

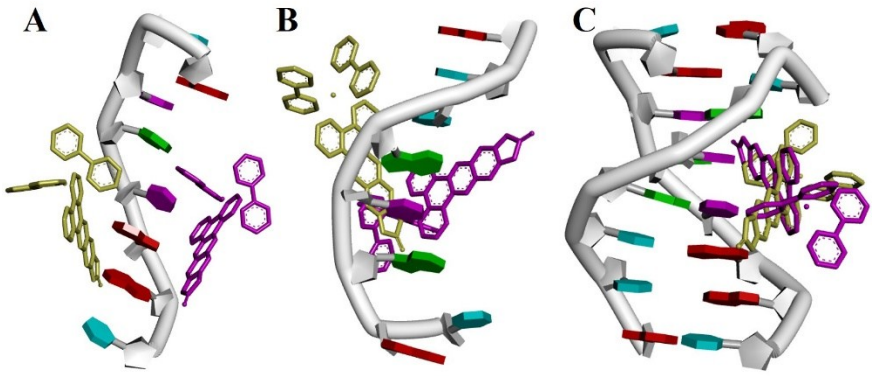


Figure S11. The calculated model of the: **Δ-1**(purple one) and **Λ-1**(yellow one) bind to A) anti-tail sequence; B) tail sequence: C) tail-pair sequence.

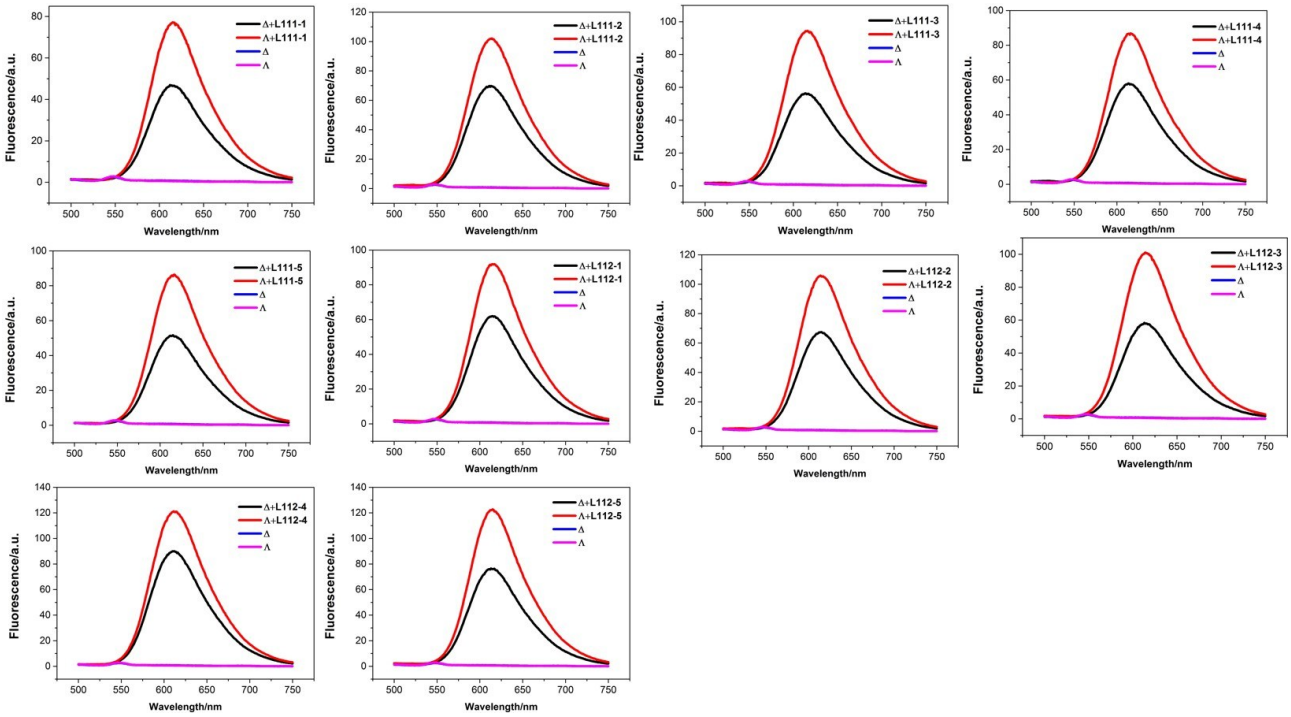


Figure S12. Comparison of emission observed for 1 μM enantiomers in the presence of 0.5 μM **L111** and **L112** with different loop-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

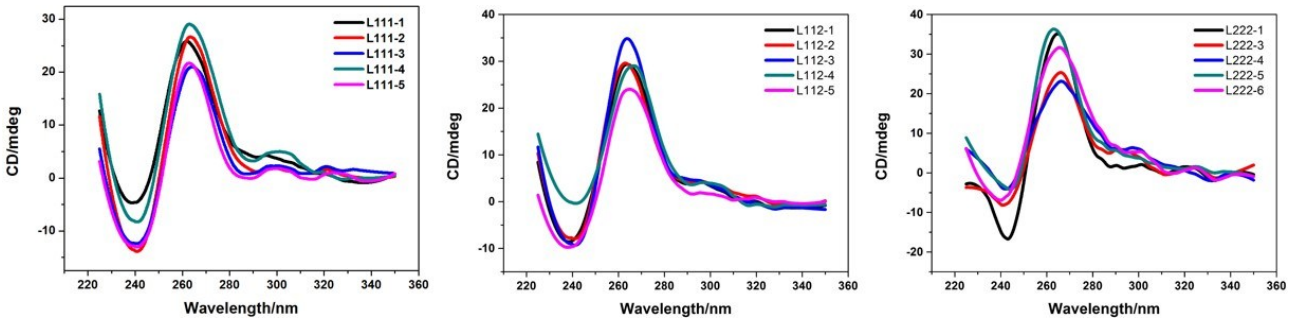


Figure S13. CD spectral of different GQs with parallel topology.

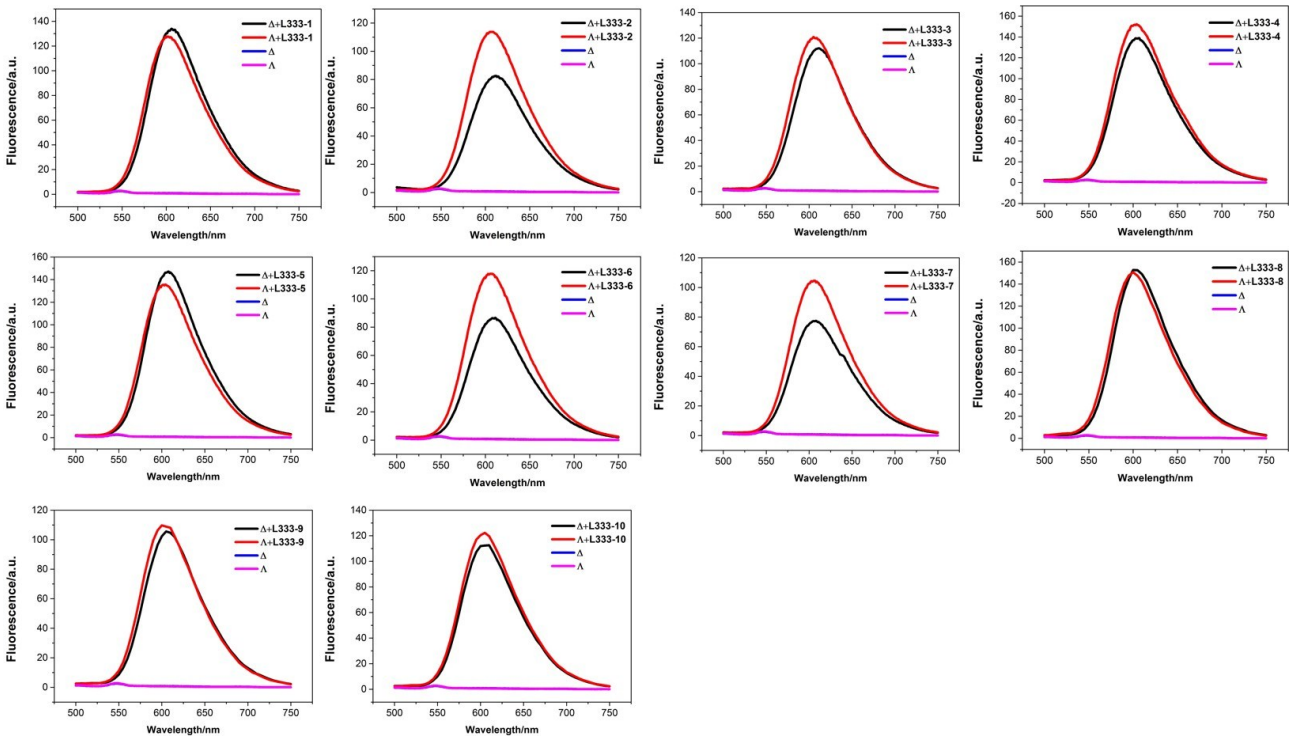


Figure S14. Comparison of emission observed for 1 μM enantiomers in the presence of 0.5 μM **L333-n** with different loop-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

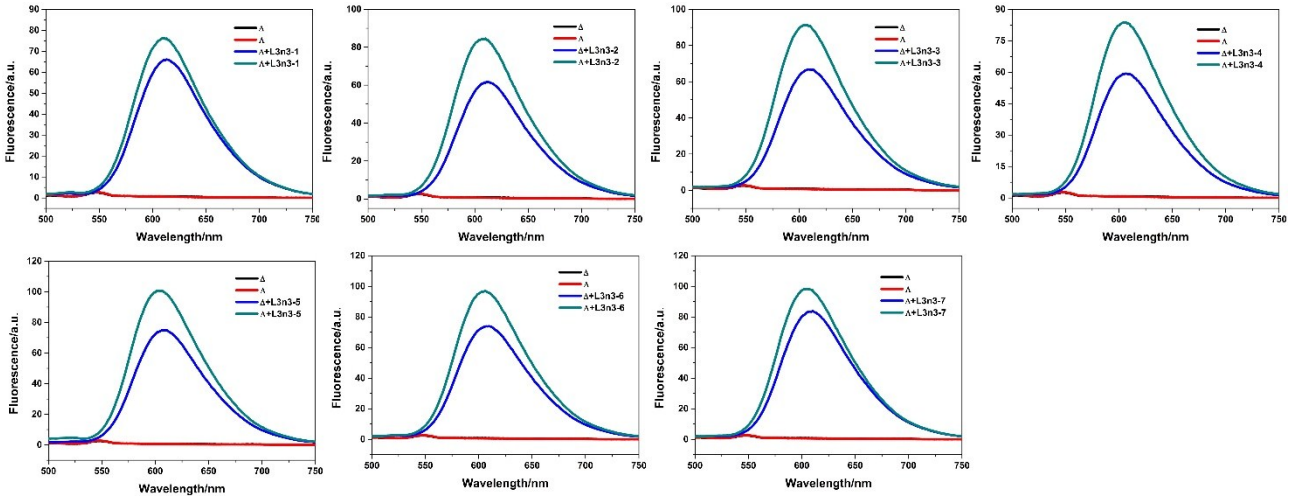


Figure S15. Comparison of emission observed for 1 μM enantiomers in the presence of 0.5 μM **L3n3** with different loop-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

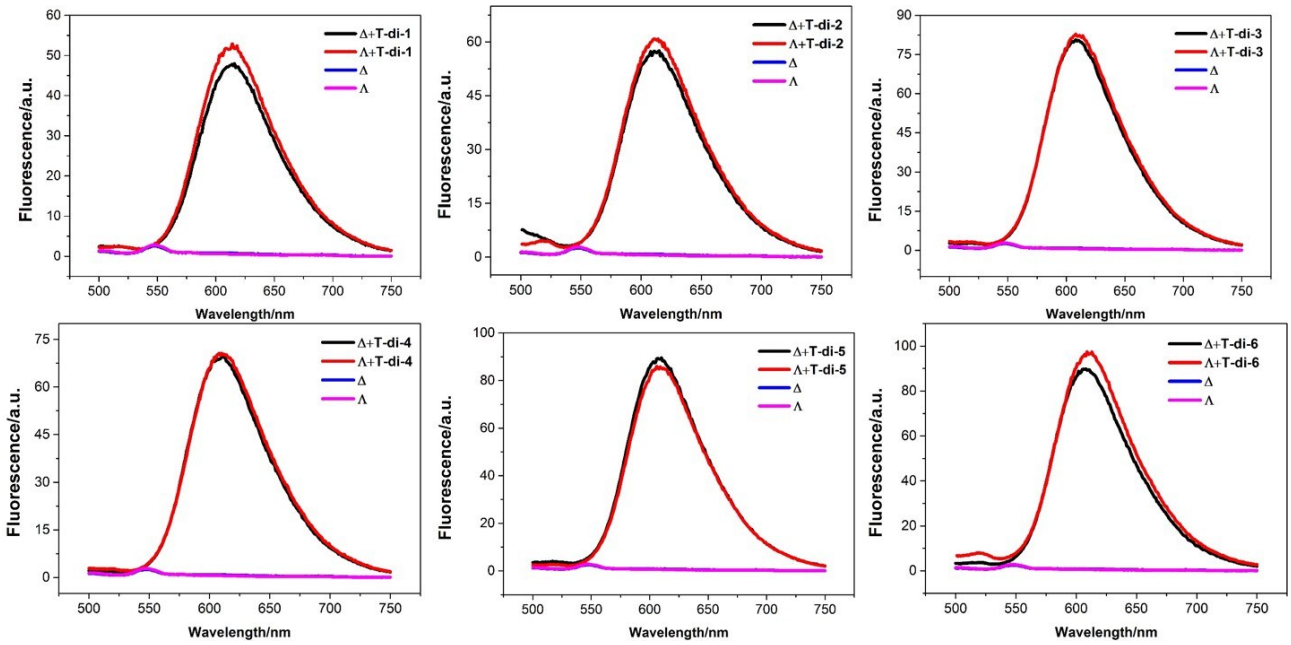


Figure S16. Comparison of emission observed for 1 μM enantiomers in the presence of 0.5 μM **T-di-n** with different link-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

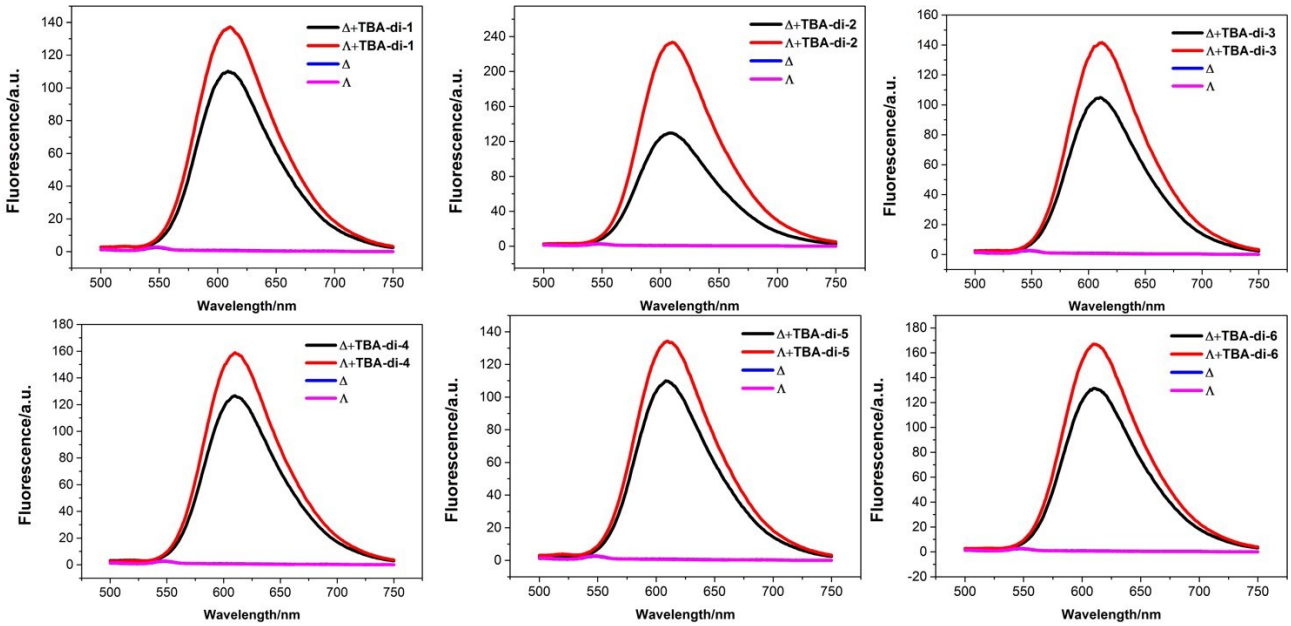


Figure S17. Comparison of emission observed for 1 μM enantiomers in the presence of 0.5 μM **TBA-di-n** with different link-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

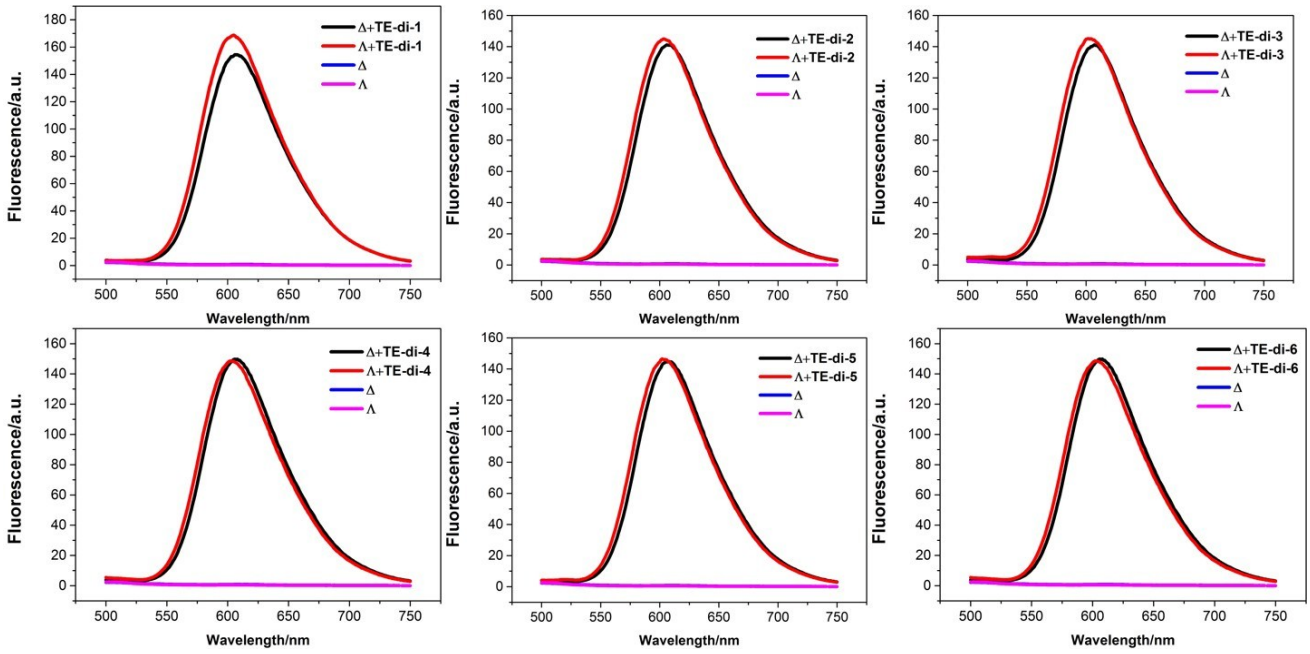


Figure S18. Comparison of emission observed for 1 μM enantiomers in the presence of 0.5 μM **TE-di-n** with different link-sequences in 10 mM Tris-HCl, 100 mM KCl buffer, pH=7.4.

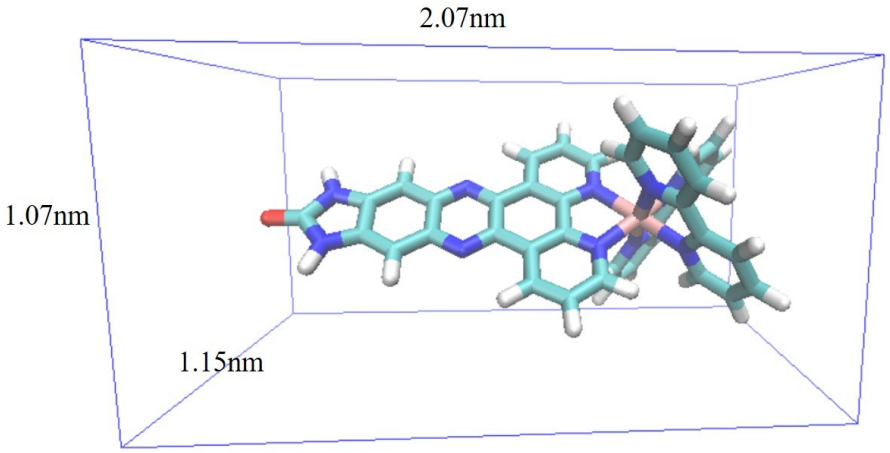
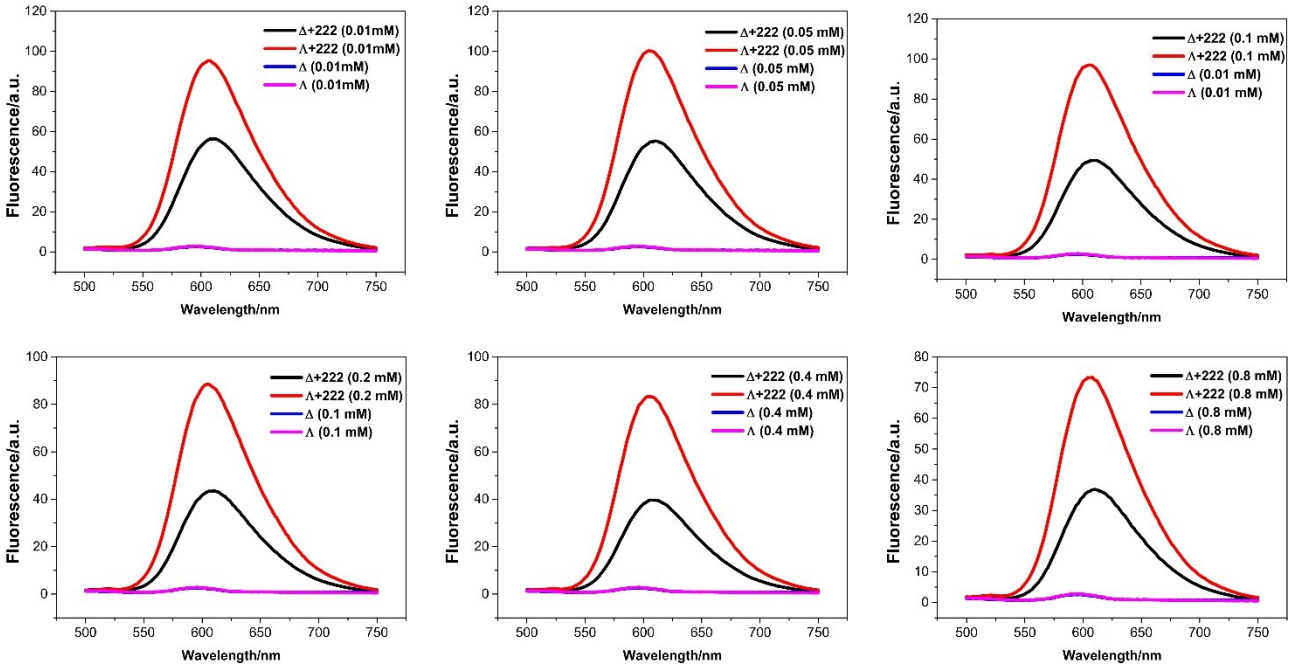


Figure S19. Cube size was calculated by Multiwfn (1). And molecular visualisation was developed using VMD on a Linux 64-bit operating system (2).



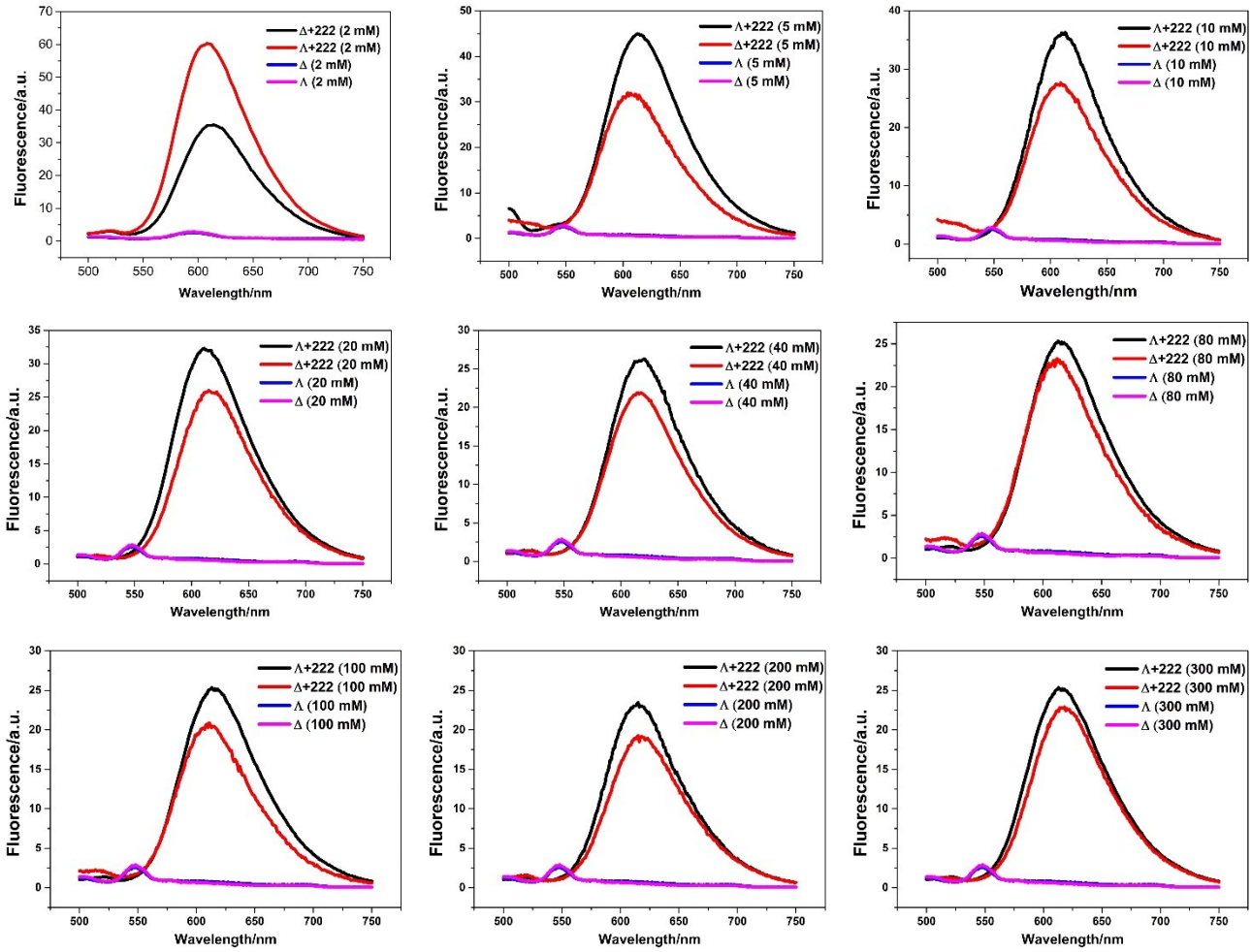


Figure S20. Comparison of emission observed for 1μM **Λ-1** in the presence of 0.5 μM **222** in 10 mM Tris-HCl, different concentration of KCl buffer, pH=7.4.

Reference

1. Tian Lu, Feiwu Chen, J. Comput. Chem. 33, 580-592 (2012)
2. Humphrey, W., Dalke, A. and Schulten, K., `VMD – Visual Molecular Dynamics', *J. Molec. Graphics* 1996, 14.1, 33-38.