

Supplementary Files

Binding studies of aloe active compounds with G-quadruplex sequences

Abhi Das, Sanjay Dutta**

Organic and Medicinal Chemistry Division,

CSIR-Indian Institute of Chemical Biology

Kolkata 700 032

TABLE OF CONTENTS

Figure S1: Absorption titration of aloe active compounds with quadruplex DNAs...Page 3.

Figure S2: Fluorescence titration of aloe active compounds with quadruplex DNAs...Page 4.

Figure S3: Thiozole orange displacement assay of aloe active compounds with quadruplex DNAs... Page 5.

Table S1: Absorption titration data for the interaction of aloe active compounds with G-quadruplex DNAs... Page 6.

Table S2: Fluorescence spectral data for the interaction of aloe active compounds with G-quadruplex DNAs... Page 7.

Table S3: Thiazole orange displacement data for the interaction of aloe active compounds with G-quadruplex DNAs... Page 8.

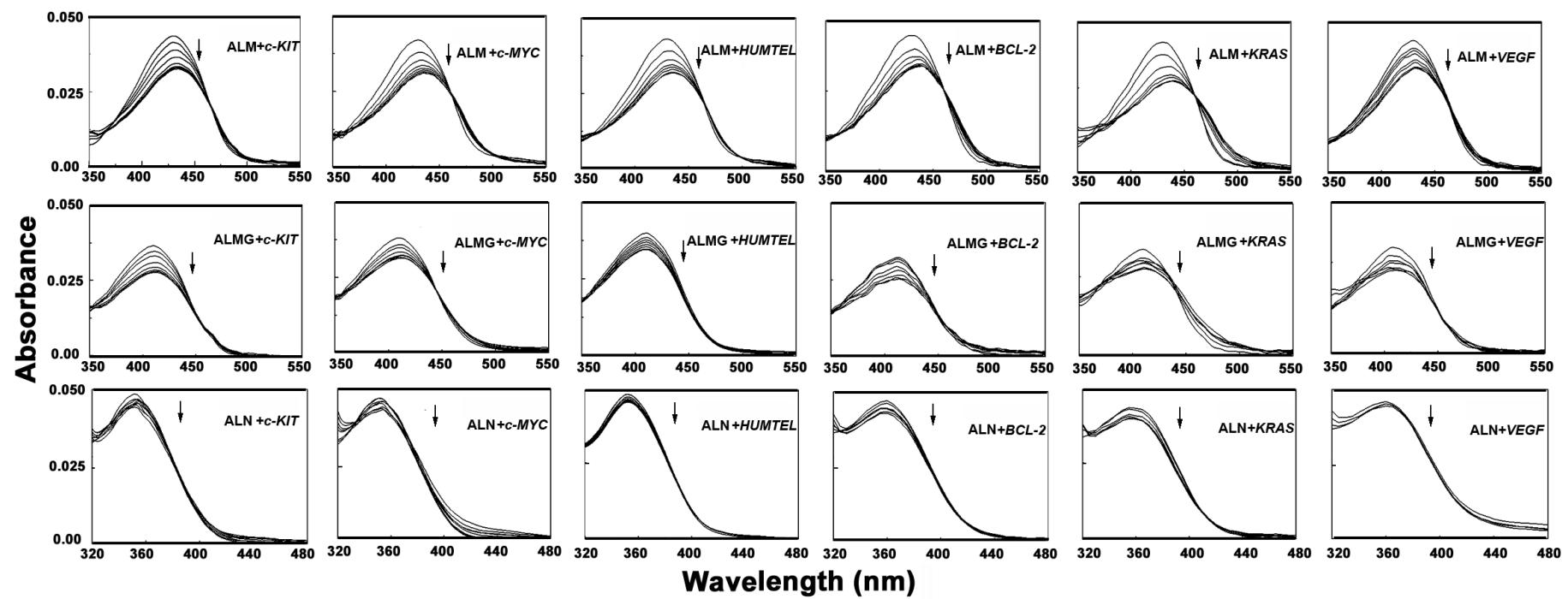


Figure S1: Absorption titration of aloe active compounds with quadruplex DNAs.

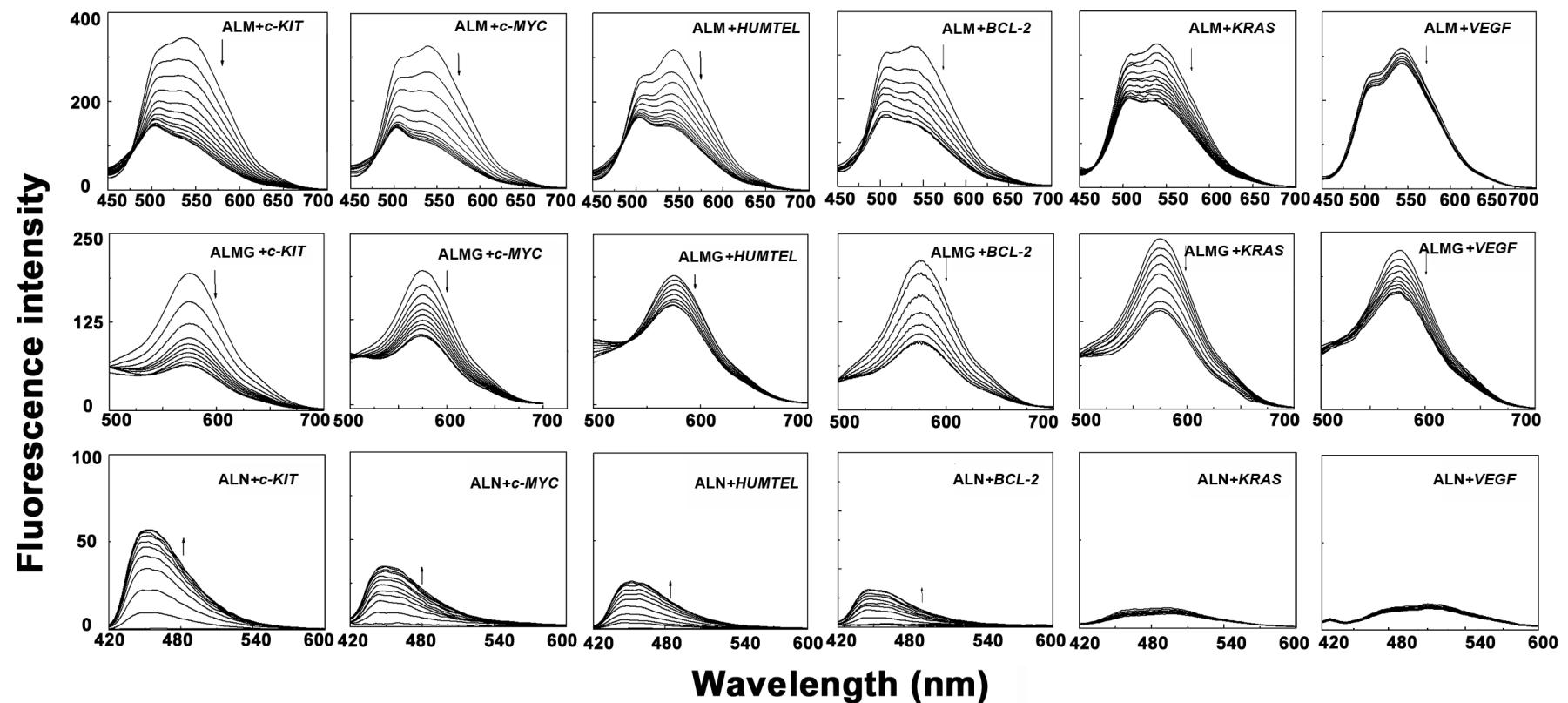


Figure S2: Fluorescence titration of aloe active compounds with quadruplex DNAs.

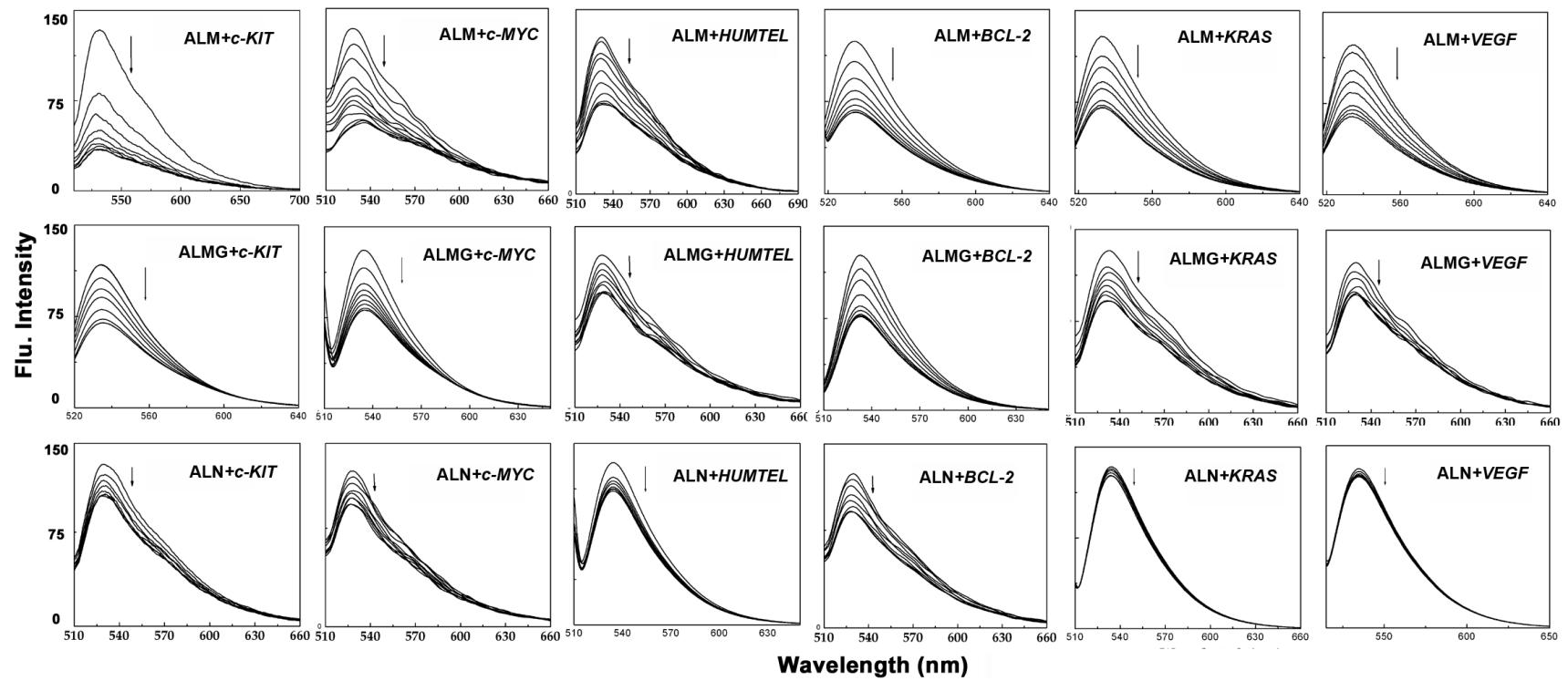


Figure S3: Thiozole orange displacement assay of aloe active compounds with quadruplex DNAs.

Table S1: Absorption titration data for the interaction of aloe active compounds with G-quadruplex DNAs.

		<i>c-KIT</i>	<i>c-MYC</i>	<i>HUMTEL</i>	<i>BCL-2</i>	<i>KRAS</i>	<i>VEGF</i>
ALM	Hypochromicity (%)	24.53	25.6	25.9	22.89	29.5	21.4
	Bathochromic shifts (nm)	4	6	4	8	10	4
	Saturating DNA/Ligand ratio	27	30	35	32	40	45
	$K_i (10^5 \text{ M}^{-1})$	2.11±0.33	1.02±0.33	0.85±0.02	0.99±0.01	0.62±0.04	0.45±0.02
	n	8.13±0.34	4.2±0.44	6.5±0.45	5.8±0.20	8.2±0.34	7.5±0.64
ALMG	Hypochromicity (%)	24	18	12.8	22.36	18.85	21.26
	Bathochromic shifts (nm)	3	0	0	0	0	0
	Saturating DNA/Ligand ratio	32	36	45	40	45	55
	$K_i (10^4 \text{ M}^{-1})$	9.70±0.50	7.78±0.25	5.20±0.82	8.40±0.25	6.40±0.33	1.23±0.24
	n	5.42±0.44	5.54±0.30	3.63±0.46	6.25±0.28	4.26±0.34	6.30±0.15
ALN	Hypochromicity (%)	6	5	4	5	4	--
	Bathochromic shifts (nm)	0	0	0	0	0	0
	Saturating DNA/Ligand ratio	--	--	-	--	--	--
	$K_{BH} (10^3 \text{ M}^{-1})$	7.23±0.50	5.30±0.35	3.30±0.48	5.68±0.66	2.10±0.32	--

Table S2: Fluorescence spectral data for the interaction of aloe active compounds with G-quadruplex DNAs.

		<i>c-KIT</i>	<i>c-MYC</i>	<i>HUMTEL</i>	<i>BCL-2</i>	<i>KRAS</i>	<i>VEGF</i>
ALM	Quenching (%)	67	66	54	53.4	38	10
	Saturating DNA/Ligand ratio	28	32	35	35	42	50
	$K_i (10^5 \text{ M}^{-1})$	2.35±0.05	2.05±0.05	0.94±0.02	1.02±0.12	0.48±0.04	0.12±0.02
ALMG	n	10.0±0.65	4.2±0.10	6.6±0.05	6.8±0.15	10.56±0.20	7.50±0.50
	Quenching (%)	67	49	22.7	55	42	26
	Saturating DNA/Ligand ratio	35	38	45	40	48	60
ALN	$K_{BH} (10^4 \text{ M}^{-1})$	8.85±0.23	8.20±0.20	2.64±0.05	8.32±0.10	7.50±0.56	2.02±0.25
	n	4.22±0.05	5.70±0.48	4.32±0.80	7.16±0.65	5.54±0.22	6.40±0.50
	$K_{BH} (10^3 \text{ M}^{-1})$	7.60±0.34	3.52±0.25	3.80±0.55	3.22±0.30	--	--

Table S3: Thiazole orange displacement data for the interaction of aloe active compounds with G-quadruplex DNAs.

		<i>c-KIT</i>	<i>c-MYC</i>	<i>HUMTEL</i>	<i>BCL-2</i>	<i>KRAS</i>	<i>VEGF</i>
ALM	TO displacement %	74.50	61.00	43.08	45.16	45.98	47.82
	K_D (μM)	2.3 \pm 0.2	4.7 \pm 0.4	12.3 \pm 0.5	11.5 \pm 0.8	22.3 \pm 0.5	23.4 \pm 0.8
ALMG	TO displacement %	40.72	38.85	24.83	37.95	30.40	24.29
	K_D (μM)	10.3 \pm 0.5	16.3 \pm 0.8	21.6 \pm 0.5	11.9 \pm 0.5	20.2 \pm 0.2	81 \pm 0.8
ALN	TO displacement %	22.08	21.43	20.38	21.13	5.94	5.27
	K_D (μM)	93.5 \pm 0.5	99.5 \pm 0.4	106.6 \pm 0.8	100.8 \pm 0.6	--	--