

Supplementary Information

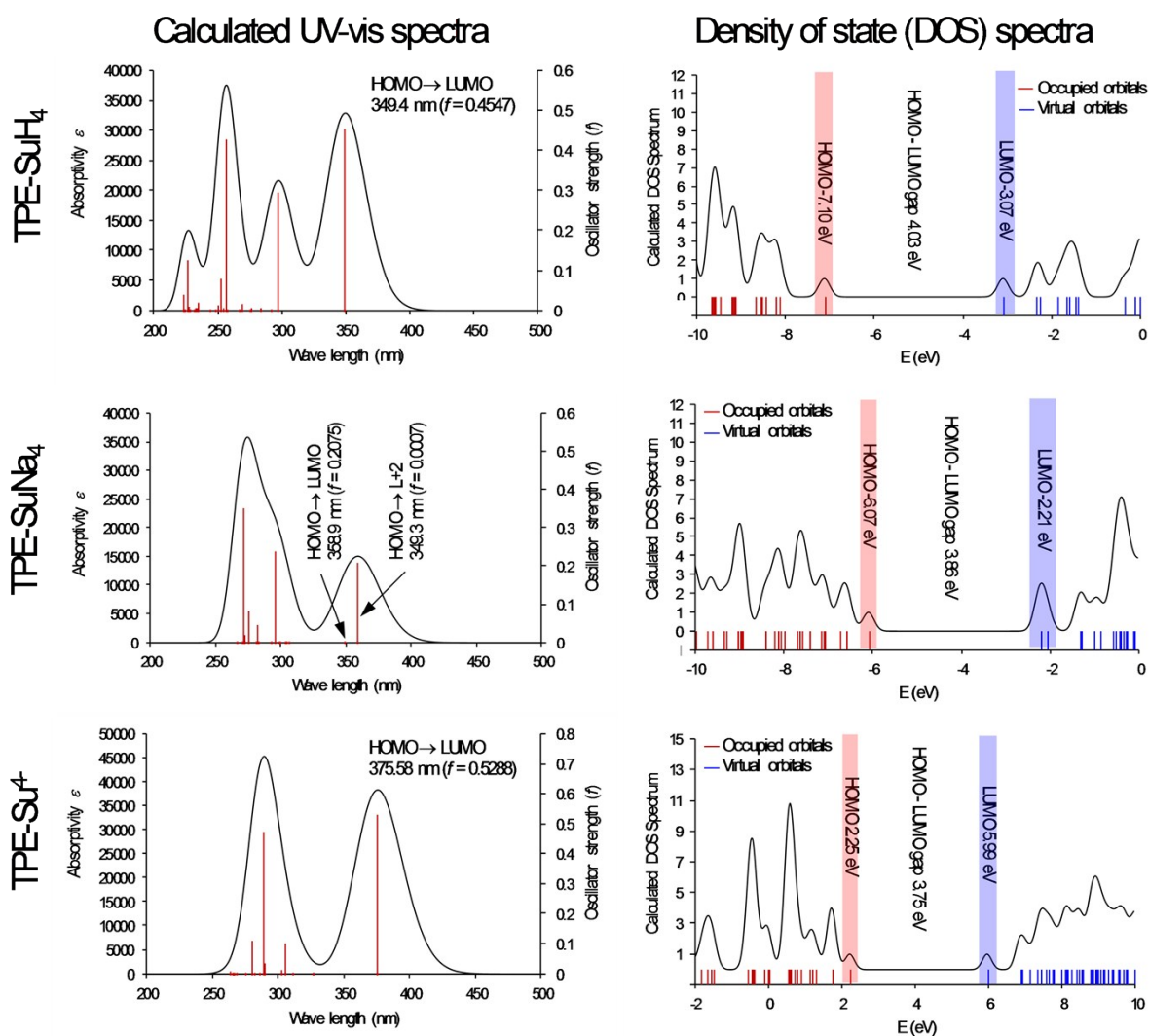


Fig. S1 The UV-vis and DOS spectra of **Su-TPE** at protonated, sodium salt and anionic states as calculated using TD-DFT at B3LYP/6-311+G(d,p) level of theory and Gauss-Sum program.

Table SI 1. Calculated Su-TPE protonated state first 25 transitions and excited states as calculated using TDDFT at 6-311+G(d,p) level of theory.

No.	λ (nm)	Osc. Strength ^f	Major contributions	Minor contributions
1	349.39	0.4547	HOMO->LUMO (99%)	
2	297.27	0.2942	HOMO->L+1 (95%)	H-5->LUMO (3%)
3	292.46	0.001	HOMO->L+2 (96%)	
4	283.60	0.0062	H-1->LUMO (75%), HOMO->L+3 (21%)	
5	276.43	0.0062	H-3->LUMO (88%)	HOMO->L+6 (7%)
6	275.16	0	H-2->LUMO (89%)	HOMO->L+7 (5%)
7	269.27	0.0168	H-1->LUMO (22%), HOMO->L+3 (67%)	H-6->LUMO (4%)
8	267.06	0.0019	H-4->LUMO (61%), HOMO->L+5 (31%)	H-5->LUMO (3%)
9	257.80	0.0002	H-7->LUMO (32%), HOMO->L+4 (61%)	HOMO->L+7 (4%)
10	256.76	0.4277	H-5->LUMO (51%), H-4->LUMO (25%), HOMO->L+5 (16%)	H-3->L+1 (2%), HOMO->L+1 (2%)
11	254.15	0.0054	H-6->LUMO (91%)	H-2->L+1 (3%), HOMO->L+3 (4%)
12	252.79	0.0775	H-5->LUMO (39%), H-4->LUMO (11%), HOMO->L+5 (38%)	H-3->L+1 (6%)
13	250.37	0.0104	HOMO->L+6 (71%)	H-4->L+1 (5%), H-3->LUMO (8%), H-1->L+2 (8%)
14	248.20	0	HOMO->L+4 (10%), HOMO->L+7 (63%)	H-6->L+1 (6%), H-4->L+2 (4%), H-2->LUMO (6%), H-1->L+1 (6%)
15	244.07	0.0002	H-7->LUMO (52%), H-1->L+1 (17%), HOMO->L+4 (21%)	HOMO->L+7 (5%)
16	235.11	0.0199	H-3->L+2 (16%), H-2->L+1 (65%)	H-7->L+5 (2%), H-5->L+7 (2%), H-1->L+6 (3%), HOMO->L+3 (5%)
17	233.95	0.0047	H-1->L+2 (65%), HOMO->L+6 (14%)	H-6->L+3 (2%), H-4->L+1 (9%), H-1->L+3 (3%)
18	232.55	0.0053	H-3->L+1 (70%), HOMO->L+5 (11%)	H-7->L+3 (3%), H-5->L+6 (3%), H-2->L+3 (2%), H-1->L+7 (2%)
19	232.16	0.0001	H-1->L+1 (67%), HOMO->L+7 (14%)	H-7->LUMO (6%), H-4->L+3 (3%)
20	228.36	0.001	H-2->L+2 (87%)	H-3->L+1 (6%)
21	227.42	0.0083	H-3->L+2 (74%), H-2->L+1 (22%)	
22	226.37	0.1246	H-12->LUMO (19%), H-8->LUMO (23%), H-4->L+1 (26%), H-1->L+2 (10%)	H-10->LUMO (9%), H-1->L+3 (3%), HOMO->L+8 (3%)
23	224.29	0.0004	H-6->L+1 (26%), H-5->L+2 (21%), H-4->L+2 (15%)	H-7->LUMO (2%), H-5->L+3 (5%), H-4->L+3 (3%), H-1->L+1 (4%), H-1->L+5 (9%), HOMO->L+7 (6%)
24	223.54	0.0372	H-8->LUMO (38%), H-4->L+1 (31%)	H-12->LUMO (3%), H-5->L+1 (2%), H-1->L+2 (9%), H-1->L+3 (7%)
25	223.04	0.0019	H-9->LUMO (91%)	H-8->L+2 (2%)

Table SI 2. Calculated Su-TPE sodium salt state first 25 transitions and excited states as calculated using TDDFT at 6-311+G(d,p) level of theory.

No.	λ (nm)	Osc. Strength ^f	Major contributions	Minor contributions
1	358.92	0.2075	HOMO->L+2 (97%)	
2	349.38	0	HOMO->LUMO (69%), HOMO->L+1 (31%)	
3	349.25	0.0007	HOMO->LUMO (30%), HOMO->L+1 (68%)	
4	306.19	0	H-2->LUMO (89%)	H-2->L+2 (3%), H-1->LUMO (7%)
5	306.16	0	H-1->L+1 (89%)	H-2->L+1 (7%), H-1->L+2 (3%)
6	304.59	0.0011	H-3->L+2 (74%), H-1->L+2 (13%)	H-2->L+2 (4%), HOMO->L+3 (4%)
7	304.07	0.0001	H-2->L+2 (67%), H-1->L+2 (27%)	H-1->L+1 (2%)
8	303.96	0	H-3->L+2 (16%), H-2->L+2 (23%), H-1->L+2 (53%)	
9	299.51	0	H-1->LUMO (92%)	H-2->LUMO (8%)
10	299.46	0	H-2->L+1 (92%)	H-1->L+1 (7%)
11	298.55	0.0002	HOMO->L+3 (91%)	H-3->L+2 (5%)
12	295.94	0.2383	HOMO->L+4 (92%)	H-4->L+2 (3%)
13	293.12	0.0004	H-3->LUMO (75%), H-3->L+1 (24%)	
14	293.05	0	H-3->LUMO (24%), H-3->L+1 (75%)	
15	282.92	0.0005	H-5->L+2 (82%), HOMO->L+5 (11%)	
16	282.54	0.0449	H-6->L+2 (25%), H-4->L+2 (67%)	HOMO->L+4 (2%)
17	281.25	0.0019	H-5->L+2 (10%), HOMO->L+5 (80%)	H-11->L+2 (3%)
18	275.58	0.0808	H-6->L+2 (42%), H-4->L+2 (12%), HOMO->L+6 (38%)	H-10->L+2 (2%)

19	272.74	0.0179	H-5->LUMO (18%), H-4->LUMO (51%), H-4->L+1 (12%)	H-6->LUMO (6%), H-5->L+1 (5%), HOMO->L+6 (4%)
20	272.70	0.002	H-5->L+1 (18%), H-4->LUMO (14%), H-4->L+1 (53%)	H-6->L+1 (6%), H-5->LUMO (5%)
21	271.40	0.3498	H-6->L+2 (27%), H-4->L+2 (14%), HOMO->L+6 (45%)	HOMO->L+4 (2%)
22	270.87	0.0002	H-5->LUMO (60%), H-4->LUMO (30%)	H-6->LUMO (7%)
23	270.83	0.0001	H-5->L+1 (61%), H-4->L+1 (30%)	H-6->L+1 (7%)
24	267.02	0	H-6->LUMO (62%), H-6->L+1 (21%), H-5->LUMO (11%)	H-5->L+1 (4%)
25	266.97	0.0004	H-6->LUMO (21%), H-6->L+1 (62%), H-5->L+1 (11%)	H-5->LUMO (3%)

Table SI 3. Calculated Su-TPE anionic state first 25 transitions and excited states as calculated using TDDFT at 6-311+G(d,p) level of theory.

No.	λ (nm)	Osc. Strength f	Major contributions	Minor contributions
1	375.58	0.5288	HOMO->LUMO (99%)	
2	327.06	0.0009	H-1->LUMO (95%)	H-2->LUMO (2%)
3	327.05	0.0007	H-2->LUMO (95%)	H-1->LUMO (2%)
4	327.04	0	H-3->LUMO (95%)	H-4->LUMO (3%)
5	327.04	0.0001	H-4->LUMO (95%)	H-3->LUMO (3%)
6	311.75	0.0001	HOMO->L+1 (94%)	
7	305.17	0.0998	H-6->LUMO (13%), HOMO->L+2 (84%)	
8	302.19	0.0113	H-5->LUMO (88%)	HOMO->L+3 (9%)
9	289.80	0.0341	H-5->LUMO (10%), HOMO->L+3 (87%)	
10	289.03	0.4746	H-6->LUMO (81%), HOMO->L+2 (12%)	HOMO->L+4 (4%)
11	286.23	0	H-7->LUMO (83%)	H-9->LUMO (9%), HOMO->L+8 (3%)
12	281.94	0.0003	H-8->LUMO (76%), HOMO->L+7 (17%)	H-5->L+1 (3%)
13	280.11	0.1081	HOMO->L+4 (81%)	H-20->LUMO (3%), H-12->LUMO (4%), H-6->LUMO (4%)
14	275.45	0	H-9->LUMO (53%), HOMO->L+5 (26%), HOMO->L+8 (11%)	H-7->LUMO (5%)
15	268.96	0.0014	H-10->LUMO (27%), HOMO->L+6 (67%)	
16	267.05	0.0003	H-3->L+2 (27%), H-1->L+1 (45%)	H-4->L+2 (5%), H-2->L+2 (4%), H-1->L+3 (6%)
17	267.05	0.0002	H-3->L+1 (48%), H-1->L+2 (34%)	H-3->L+3 (7%), H-2->L+2 (3%), H-1->L+4 (2%)
18	267.05	0.0008	H-4->L+1 (11%), H-2->L+1 (34%), H-2->L+2 (21%)	H-4->L+2 (7%), H-3->L+2 (9%), H-2->L+3 (5%), H-1->L+1 (3%)
19	267.03	0.0006	H-4->L+1 (35%), H-4->L+2 (26%), H-2->L+1 (13%), H-2->L+2 (10%)	H-4->L+3 (5%)
20	266.26	0	H-9->LUMO (17%), HOMO->L+5 (67%)	H-7->LUMO (7%), HOMO->L+8 (3%)
21	265.48	0.0001	H-3->L+2 (39%), H-1->L+1 (34%)	H-3->L+4 (3%), H-2->L+1 (6%), H-1->L+3 (8%), H-1->L+7 (2%)
22	265.48	0.0001	H-4->L+2 (35%), H-2->L+1 (34%)	H-4->L+4 (3%), H-2->L+2 (3%), H-2->L+3 (8%), H-2->L+7 (2%), H-1->L+1 (7%)
23	265.47	0	H-4->L+1 (14%), H-3->L+1 (27%), H-2->L+2 (25%), H-1->L+2 (13%)	H-4->L+3 (4%), H-3->L+3 (6%)
24	265.46	0	H-4->L+1 (26%), H-3->L+1 (15%), H-2->L+2 (11%), H-1->L+2 (26%)	H-4->L+3 (6%), H-3->L+3 (4%), H-1->L+4 (2%)
25	263.47	0.0076	H-10->LUMO (64%), HOMO->L+6 (30%)	

Dynamic light scattering

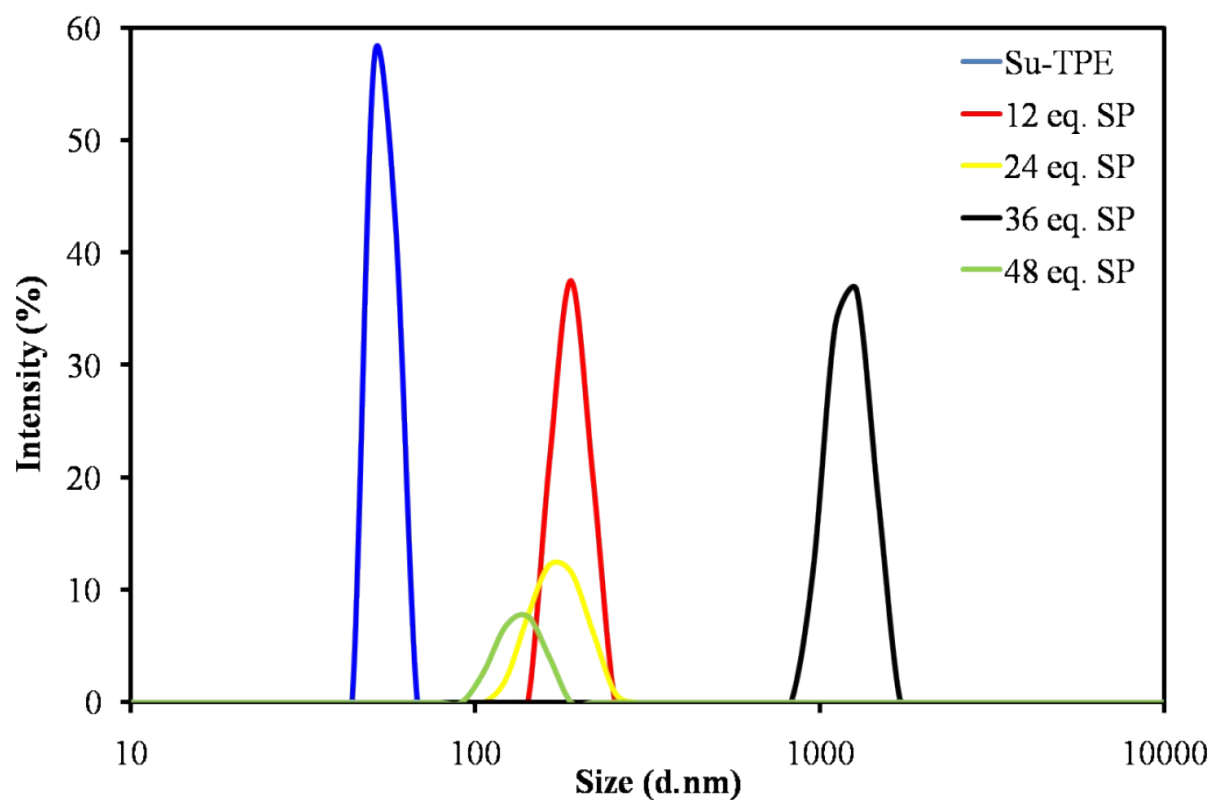


Fig. S2 DLS of **Su-TPE** at pH 7 with the addition of spermine (12, 18, 24, 36 and 48 equiv.)

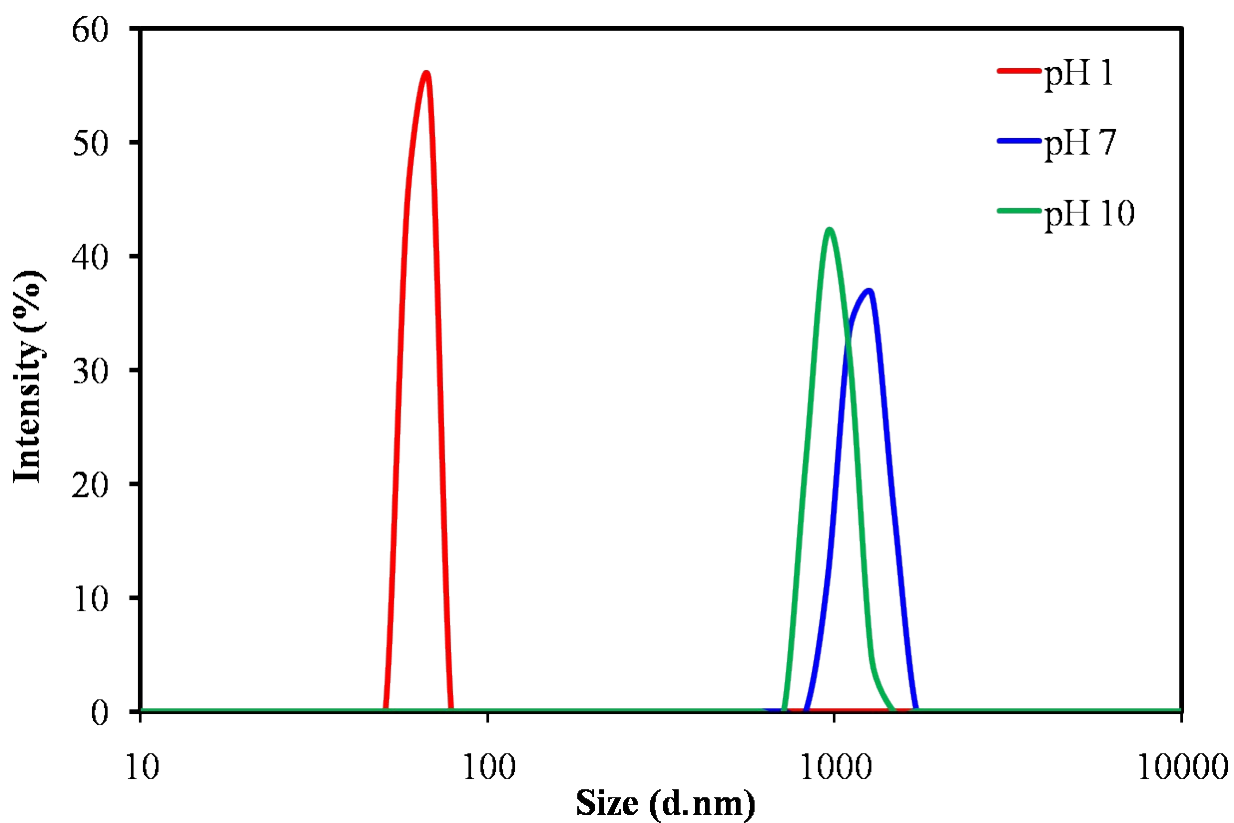


Fig. S3 DLS of **Su-TPE** at pH 1, 7 and 10 with the addition of spermine (36 equiv.)

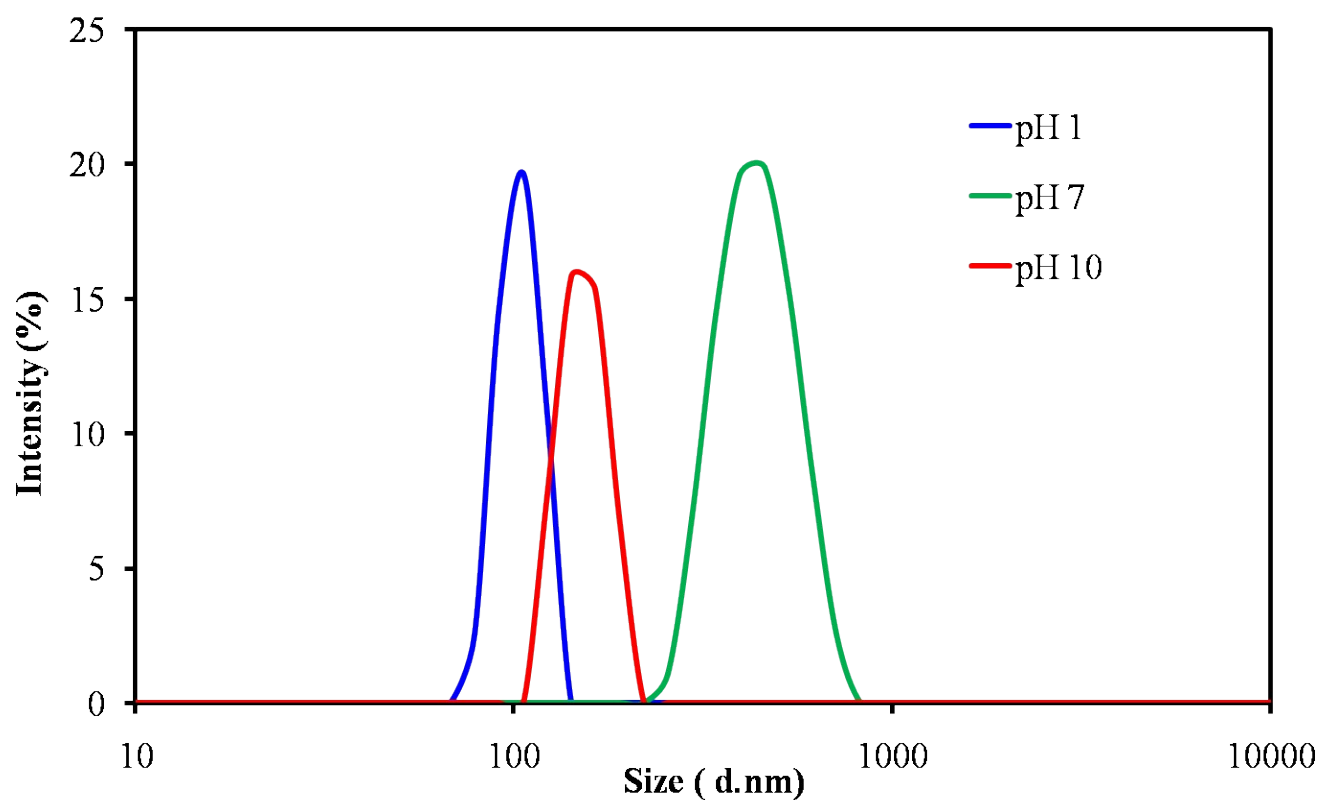


Fig. S4 DLS of **Su-TPE** at pH 1, 7 and 10 with the addition of spermine (36 equiv.)

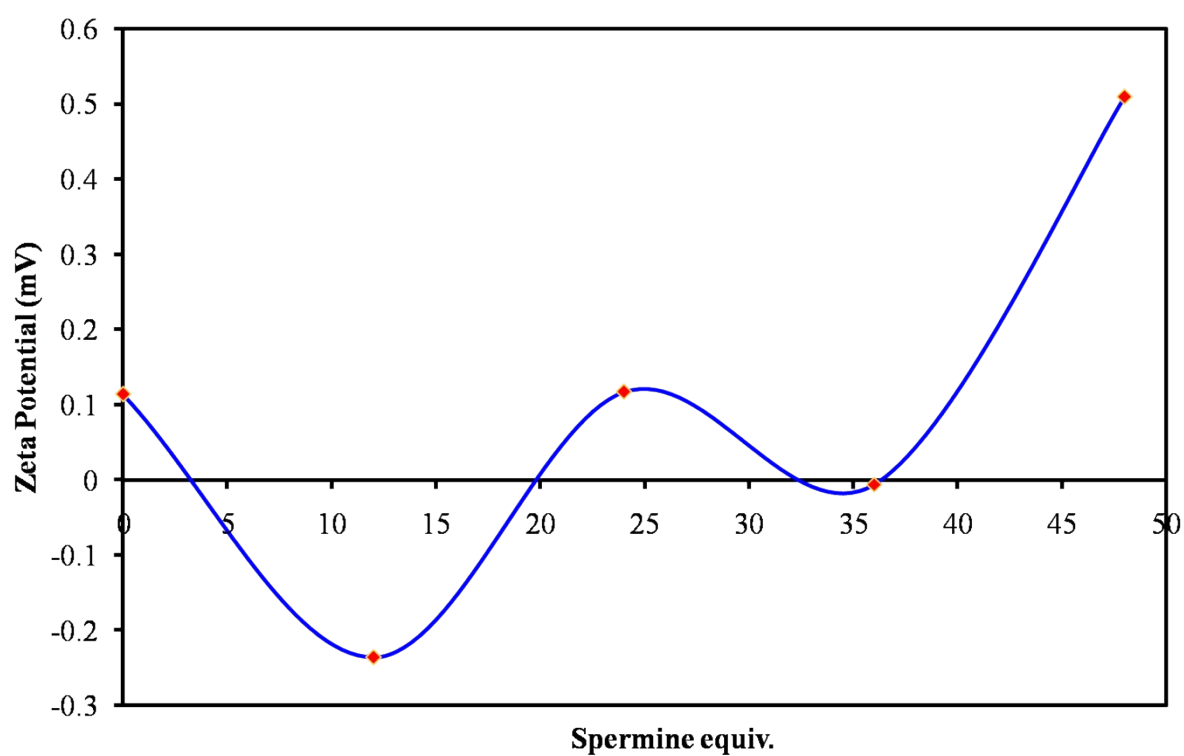


Fig. S5 Zeta potential of **Su-TPE** at pH 7 with the addition of spermine (12, 18, 24, 36 and 48 equiv.).

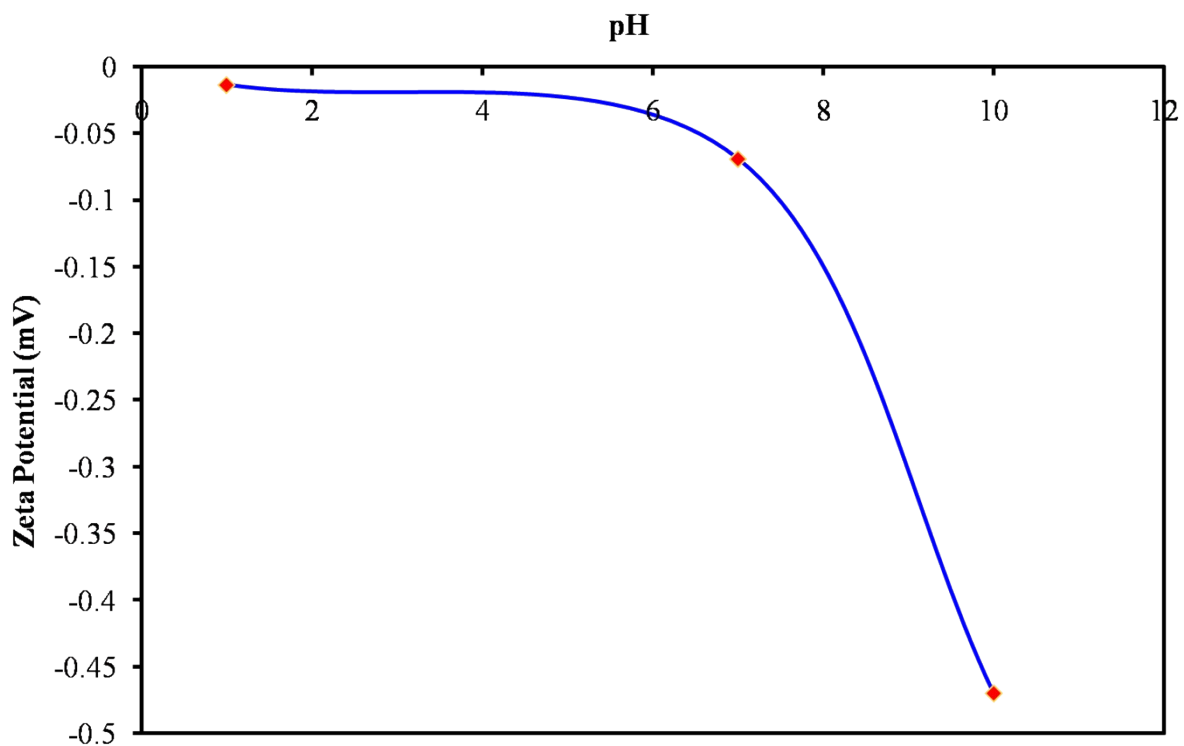


Fig. S6 Zeta potential of **Su-TPE** at pH 1, 7 and 10 with the addition of spermine (36 equiv.).

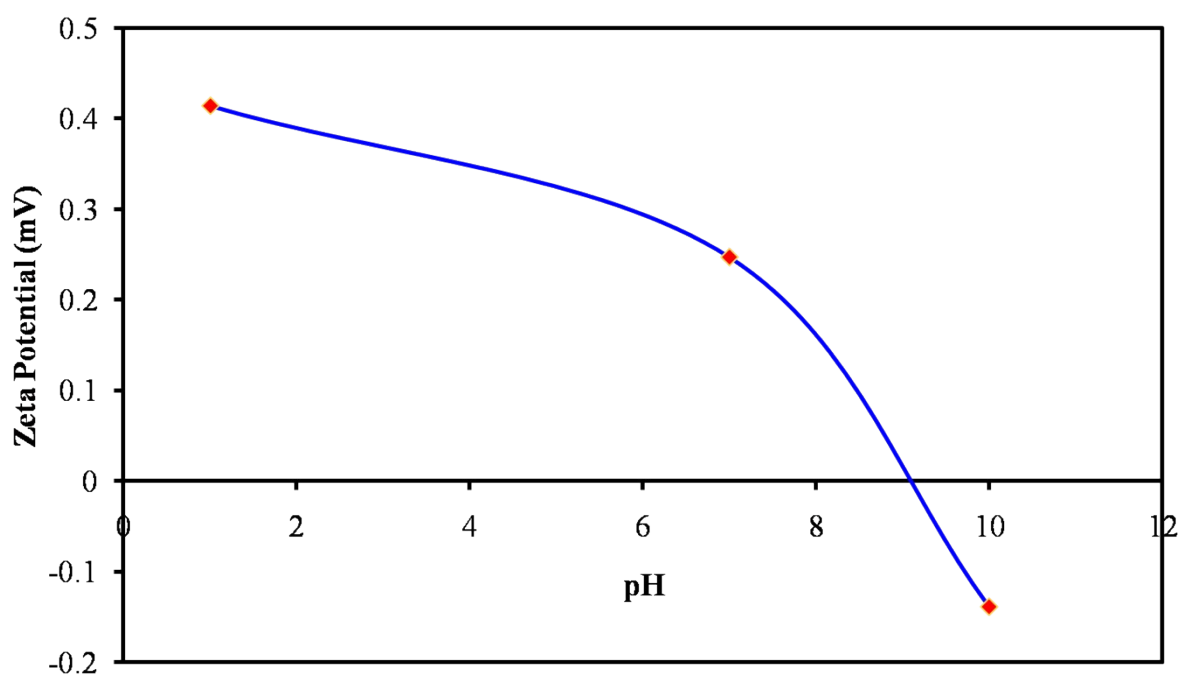


Fig. S7 Zeta potential of **Su-TPE** at pH 1, 7 and 10 with the addition of spermine (48 equiv.).