

Supporting Information

Modulating the Substrate Selectivity of DNA Aptamers using Surfactants

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Table S1. Partitioning coefficients ($\log D$) generated using the ChemAxon $\log D$ calculator. All values calculated for pH= 7.4.

Steroid	$\log D$
DIS	1.04
DOA	3.77
DCA	1.15
BE	3.75

Table S2. Chemical supplier information.

Chemical	Supplier	Catalog Number	Purity/ Composition
Triton X-100	CalBioChem	648466	-
Tween 20	Sigma Life Sciences	P1379	47% Lauric acid
Sodium dodecyl sulfate (SDS)	Research Products International Group	L22010	≥99%
Cetyl trimethylammonium bromide (CTAB)	Sigma Aldrich	H5882	≥98%
3-[(3-cholamidopropyl)dimethylammonio]-1-propanesulfonate (CHAPS)	Sigma Aldrich	C3023	98%
Dehydroisoandrosterone 3-sulfate sodium salt dihydrate (DIS)	Sigma Aldrich	D5297	≥98%
Deoxycholic acid sodium salt (DCA)	Sigma Aldrich	30170	≥98%
Beta-Estradiol (BE)	Sigma Aldrich	E8875	≥98%
Deoxycorticosterone acetate (DOA)	Sigma Aldrich	D7000	97.8%

Table S3. Tabular data for the average percent displacement (% dis.) and standard deviation (s.d.) for three trials using the DIS biosensor in the presence of various surfactants.

[DIS] (μM)	buffer		SDS		CTAB	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	19.29	0.92	21.02	0.44	2.64	0.24
1111	19.06	0.58	15.87	0.39	1.33	0.07
370	15.00	0.47	10.65	0.26	1.96	0.10
123	11.01	0.41	6.62	0.19	2.03	0.10
41.2	6.28	0.19	3.16	0.23	1.91	0.07
13.7	3.01	0.09	2.06	0.05	1.89	0.08
4.57	1.39	0.05	1.06	0.03	1.97	0.06
1.52	0.72	0.03	1.49	0.05	1.76	0.07

[DIS] (μM)	CHAPS		Tween 20		Triton X-100	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	7.32	0.13	21.32	0.72	18.31	0.44
1111	3.93	0.09	16.18	0.42	12.61	0.45
370	2.56	0.06	10.12	0.18	7.07	0.03
123	2.02	0.06	5.78	0.12	3.78	0.07
41.2	2.35	0.04	2.94	0.08	1.93	0.06
13.7	1.64	0.03	1.48	0.05	1.25	0.04
4.57	1.81	0.05	0.82	0.03	0.89	0.03
1.52	1.47	0.05	0.40	0.01	0.85	0.03

Table S4. Tabular data for the average percent displacement (% dis.) and standard deviation (s.d.) for three trials using the DIS aptamer at various SDS concentrations with DOA or DIS as the ligand.

[DOA] (μM)	0 % SDS		0.01% SDS		1 % SDS		4 % SDS	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	4.98	1.64	0.43	1.44	0.35	2.48	-0.24	1.72
1111	8.34	1.33	6.01	1.40	-0.20	2.12	-0.43	2.07
370	11.38	1.04	11.52	1.34	0.40	2.28	-0.39	1.33
123	13.11	1.10	12.12	1.60	-0.29	1.62	-0.09	1.77
41.2	10.15	0.92	9.38	0.13	-1.27	2.23	-1.09	0.46
13.7	5.93	0.74	5.57	0.77	-0.73	2.31	-0.29	1.48
4.57	2.32	1.10	2.80	0.84	-0.26	2.09	0.17	1.40
1.52	0.83	1.06	1.34	1.15	-0.97	1.87	-0.40	1.54

[DIS] (μM)	0 % SDS		0.01% SDS		1 % SDS		4 % SDS	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	19.27	1.55	22.07	1.46	18.54	2.94	16.49	2.23
1111	17.43	0.82	18.14	1.32	15.34	2.86	12.44	2.77
370	13.67	1.68	12.87	1.55	10.09	2.95	6.46	1.20
123	9.11	1.04	8.69	1.07	4.37	2.98	2.78	1.08
41.2	5.00	0.49	4.29	0.96	0.71	2.06	1.26	1.54
13.7	1.63	0.87	1.51	0.80	0.10	2.01	-0.16	1.22
4.57	0.82	0.85	0.82	0.79	-0.70	2.10	0.21	1.43
1.52	0.81	1.06	0.11	0.86	-0.48	2.87	-0.09	1.75

Table S5. Tabular data for the average percent displacement (% dis.) and standard deviation (s.d.) for three trials using the DCA aptamer at various SDS concentrations with DCA or DIS as the ligand.

[DCA] (μM)	0 % SDS		0.01% SDS		1 % SDS		4 % SDS	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	26.01	1.16	36.78	2.05	16.10	2.03	9.57	1.45
1111	23.66	2.50	33.52	3.15	8.37	2.74	3.68	2.64
370	23.18	3.93	29.87	4.37	3.22	1.47	2.78	1.64
123	20.66	0.81	22.72	6.70	1.59	1.62	1.47	1.13
41.2	12.89	1.51	14.77	2.40	0.40	1.69	0.77	2.58
13.7	6.54	1.87	7.10	2.91	-0.36	2.15	1.37	1.78
4.57	1.99	1.11	3.19	1.30	0.17	1.79	1.83	2.62
1.52	0.59	1.04	0.70	1.99	1.52	2.00	1.93	2.11

[DIS] (μM)	0 % SDS		0.01% SDS		1 % SDS		4 % SDS	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	38.73	2.63	44.36	4.34	41.45	2.84	30.43	3.29
1111	33.87	4.41	39.97	3.50	29.24	3.19	20.45	2.96
370	21.15	2.51	25.96	2.70	17.22	2.25	9.18	2.74
123	10.40	1.19	12.55	1.14	7.16	1.71	4.03	2.31
41.2	3.90	1.03	3.10	4.19	1.43	2.86	0.49	1.00
13.7	0.58	1.00	1.27	1.29	1.33	1.85	0.14	0.64
4.57	-0.08	1.08	0.75	0.73	0.04	1.12	-0.50	1.52
1.52	-0.16	0.65	-0.45	1.60	0.60	1.42	-0.89	1.46

Table S6. Tabular data for the average percent displacement (% dis.) and standard deviation (s.d.) for three trials using the BE aptamer at various SDS concentrations with BE or DIS as the ligand.

[BE] (μM)	0 % SDS		0.01% SDS		1 % SDS		4 % SDS	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	10.41	0.96	18.52	1.70	13.00	2.00	9.73	0.32
1111	11.97	1.03	14.05	0.24	8.24	0.30	5.31	0.27
370	12.84	0.23	13.01	0.33	6.04	0.64	2.16	0.28
123	12.89	0.36	11.25	0.29	3.25	0.05	1.46	0.10
41.2	15.93	1.87	12.83	0.51	1.34	0.32	0.65	0.15
13.7	9.27	0.63	8.59	0.04	1.08	0.02	1.54	0.47
4.57	4.50	0.51	4.72	0.12	1.06	0.11	1.35	0.12
1.52	2.11	0.20	2.15	0.06	0.60	0.10	1.18	0.07

[DIS] (μM)	0 % SDS		0.01% SDS		1 % SDS		4 % SDS	
	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.	% dis.	s.d.
3333	21.70	1.11	22.68	0.56	15.86	0.91	10.21	0.67
1111	12.42	0.22	13.16	0.24	8.86	0.12	5.15	0.57
370	6.03	0.14	6.36	0.16	4.40	0.37	2.63	0.08
123	2.77	0.08	3.14	0.13	1.76	0.10	1.59	0.25
41.2	1.67	0.44	1.83	0.15	1.04	0.23	1.09	0.17
13.7	0.74	0.19	1.11	0.07	1.04	0.03	1.45	0.22
4.57	0.62	0.11	0.93	0.14	0.82	0.09	1.98	0.21
1.52	1.03	0.10	0.85	0.08	1.43	0.09	1.14	0.22