

Supplementary Information

**Development of aptasensor for dibutyl phthalate detection and the elucidation of assay
inhibition factors**

*Hyerin Song, Hyun Jeong Lim, and *Ahjeong Son*

Department of Environmental Science and Engineering, Ewha Womans University, Seoul
03760, Republic of Korea

*Corresponding Author (A. Son): 52 Ewhayeodae-gil, Seodaemun-gu, Ewha Womans
University, Seoul 03760, Republic of Korea; E-mail. ason@ewha.ac.kr,
ahjeong.son@gmail.com; Phone. +82 (2) 3277-3339

LIST OF FIGURES & TABLES

Figure S1. (a) The fluorescence intensities depending on various combinations with aptamer, probe, SYBR Green I, and DBP. (b) Comparison of fluorescence intensity between aptamer and truncated aptamer.

Figure S2. Decrease ratio in the experiments based on time.

Table S1. List of compounds that were used for the selectivity verification

Table S2. *P*-values (t-test) for selectivity of SG-aptasensor

Table S3. *P*-values (t-test) for temperature experiment of SG-aptasensor

Table S4. Studies for the existence of PAEs in various environmental matrixes.

Table S5. List of precision (%RSD, Relative Standard Deviation)

Table S6. % inhibition for Figure 5

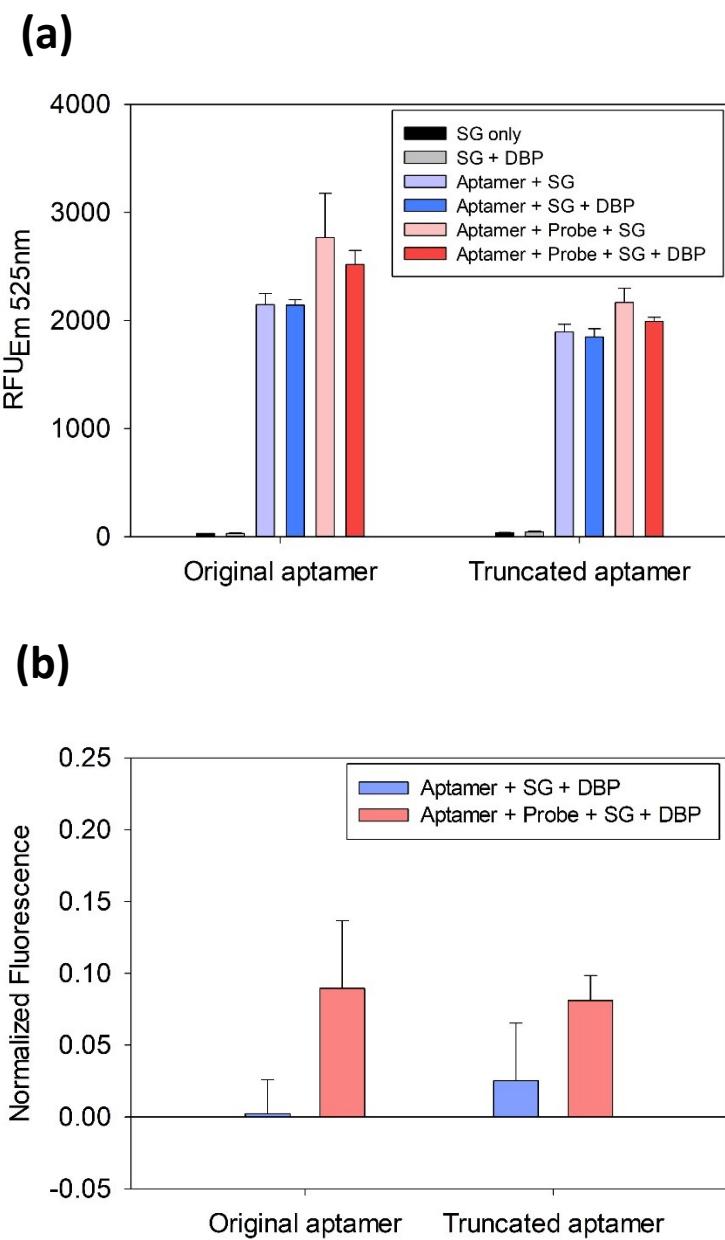


Figure S1

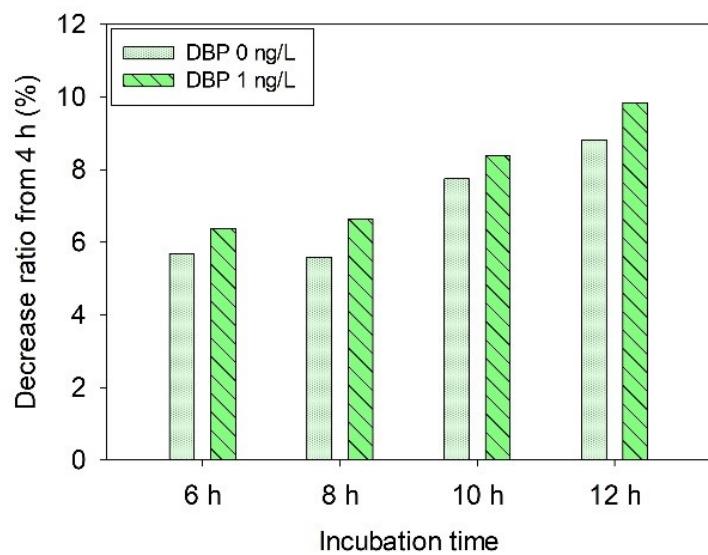


Figure S2

Name (Abbr.)	Molecular structure	Chemical formula	M.W	Solubility in water
Dibutyl phthalate (DBP)		C ₁₆ H ₂₂ O ₄	278.348 g/mol	13 mg/L (20°C)
Nonylphenol ethoxylate (NPE)*		C ₁₅ H ₂₄ O(C ₂ H ₄ O) _n	1,980 g/mol (70% in H ₂ O)	0.025 mg/L (25°C)
Triclosan (TCS)		C ₁₂ H ₇ Cl ₃ O ₂	289.50 g/mol	10 mg/L (20°C)
Bisphenol A (BPA)		C ₁₅ H ₁₆ Cl ₂	228.291 g/mol	120-300 mg/L (25°C)
Bisphenol S (BPS)		C ₁₂ H ₁₀ O ₄ S	250.27 g/mol	1100 mg/L (25°C)

Table S1. List of compounds that were used for the selectivity verification

* Tergitol-type NP-40 (nonyl phenoxypolyethoxylethanol)

Table S2. *P*-values (t-test) for selectivity of SG-aptasensor

Concentration	DBP	NPE	TCS	BPA	BPS
0 ng/L and 1 ng/L	0.0058	0.274	0.204	0.259	0.488

Table S3. *P*-values (t-test) for temperature experiment of SG-aptasensor

Temperature	2 °C	13 °C	25 °C	37 °C
2 °C		0.116	0.229	0.0005
13 °C	0.116		0.258	0.008
25 °C	0.229	0.258		0.00004
37 °C	0.0005	0.008	0.00004	

Table S4. Studies for the existence of PAEs in various environmental matrixes.

Matrix	Location	PAEs	Concentration ($\mu\text{g/L}$, ppb)	References
Water	Lake in Guangzhou city (China)	DBP DIBP DEHP	2.03 0.47 0.24	(Zeng et al. 2008)
	Manzanares and Jarama river (Spain)	DBP	0.82	(Domínguez- Morueco et al. 2014)
	Surface water in Northern industrial area (Sweden)	DBP DEP DMP BBP	6.8 0.63 0.40 0.17	(Bastos et al. 2012)
Soil or sediment	Agricultural paddy soils in Sanjiang Plain (China)	DEHP	0.22	(Wang et al. 2017)
		DBP DEP	0.16 0.06	
Air	Urban home (Japan)	DBP DEHP DEP DCHP	750 320 140 120	(Otake et al. 2004)
		BBP	20	
		DEP	45	
	California county (USA)	DIBP DBP DEHP	44.5 31.5 3.65	(Lunderberg et al. 2019)

Table S5. List of precision (%RSD, Relative Standard Deviation)

Sensitivity (Figure 2B)

DBP concentration (ng/L)	Fluorescence intensity	Normalized fluorescence intensity
0	3.3	
0.1	1.9	60.3
0.5	0.5	11.1
1	0.6	7.4
5	1.0	10.8
10	2.4	22.3
50	0.7	6.4
100	5.1	26.5

Table S6. % inhibition for Figure 5

Ions	Fs Conc. (mM)	DBP 0 ng/L	DBP 1 ng/L
Mg^{2+}	0.01 mM	1.17%	-0.77%
	0.1 mM	1.31%	3.42%
	1 mM	-1.64%	2.94%
	10 mM	-4.07%	-0.88%
	100 mM	5.29%	13.43%
Ca^{2+}	0.01 mM	10.64%	10.07%
	0.1 mM	12.85%	5.22%
	1 mM	14.99%	12.06%
	10 mM	10.77%	9.02%
	100 mM	3.05%	2.45%
Cu^{2+}	0.01 mM	3.35%	4.26%
	0.1 mM	12.00%	9.80%
	1 mM	19.72%	20.96%
	10 mM	59.68%	62.84%
	100 mM	99.06%	98.82%

Note) % Inhibition = $(F_c - F_s)/F_c * 100$, $F_c = 0$ mM

References

- (1) Feng Zeng, Kunyan Cui, Zhiyong Xie, Min Liu, Yangjie Li, Yujun Lin, Zunxiang Zeng, Fangbai Li. "Occurrence of phthalate esters in water and sediment of urban lakes in a subtropical city, Guangzhou, South China." *Environment International* 34.3 (2008): 372-380.
- (2) N. Domínguez-Morueco, S. González-Alonso, and Y. Valcárcel. "Phthalate occurrence in rivers and tap water from central Spain." *Science of the total environment* 500 (2014): 139-146.
- (2) Patricia Moreira Bastos, and Peter Haglund. "The use of comprehensive two-dimensional gas chromatography and structure-activity modeling for screening and preliminary risk assessment of organic contaminants in soil, sediment, and surface water." *Journal of Soils and Sediments* 12 (2012): 1079-1088.
- (4) He Wang, Hong Liang, and Da-Wen Gao. "Occurrence and risk assessment of phthalate esters (PAEs) in agricultural soils of the Sanjiang Plain, northeast China." *Environmental Science and Pollution Research* 24 (2017): 19723-19732.
- (5) Takamitsu Otake, Jun Yoshinaga, and Yukio Yanagisawa. "Exposure to phthalate esters from indoor environment." *Journal of Exposure Science & Environmental Epidemiology* 14.7 (2004): 524-528.
- (6) David M. Lunderberg*, Kasper Kristensen, Yingjun Liu, Pawel K. Misztal, Yilin Tian, Caleb Arata, Rebecca Wernis, Nathan Kreisberg, William W. Nazaroff, and Allen H. Goldstein. "Characterizing airborne phthalate concentrations and dynamics in a normally occupied residence." *Environmental science & technology* 53.13 (2019): 7337-7346.