

Supporting information

Electrospun Nanofibrous Membrane-based colorimetric device for rapid and simple screening of amphetamine-type stimulants in drinks

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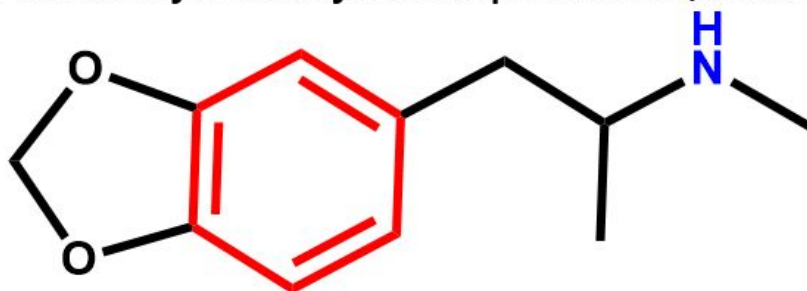
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(a) 3,4-Methylenedioxyamphetamine (MDMA)



(b) Methamphetamine

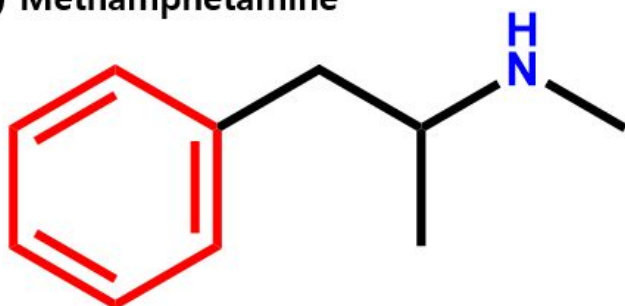


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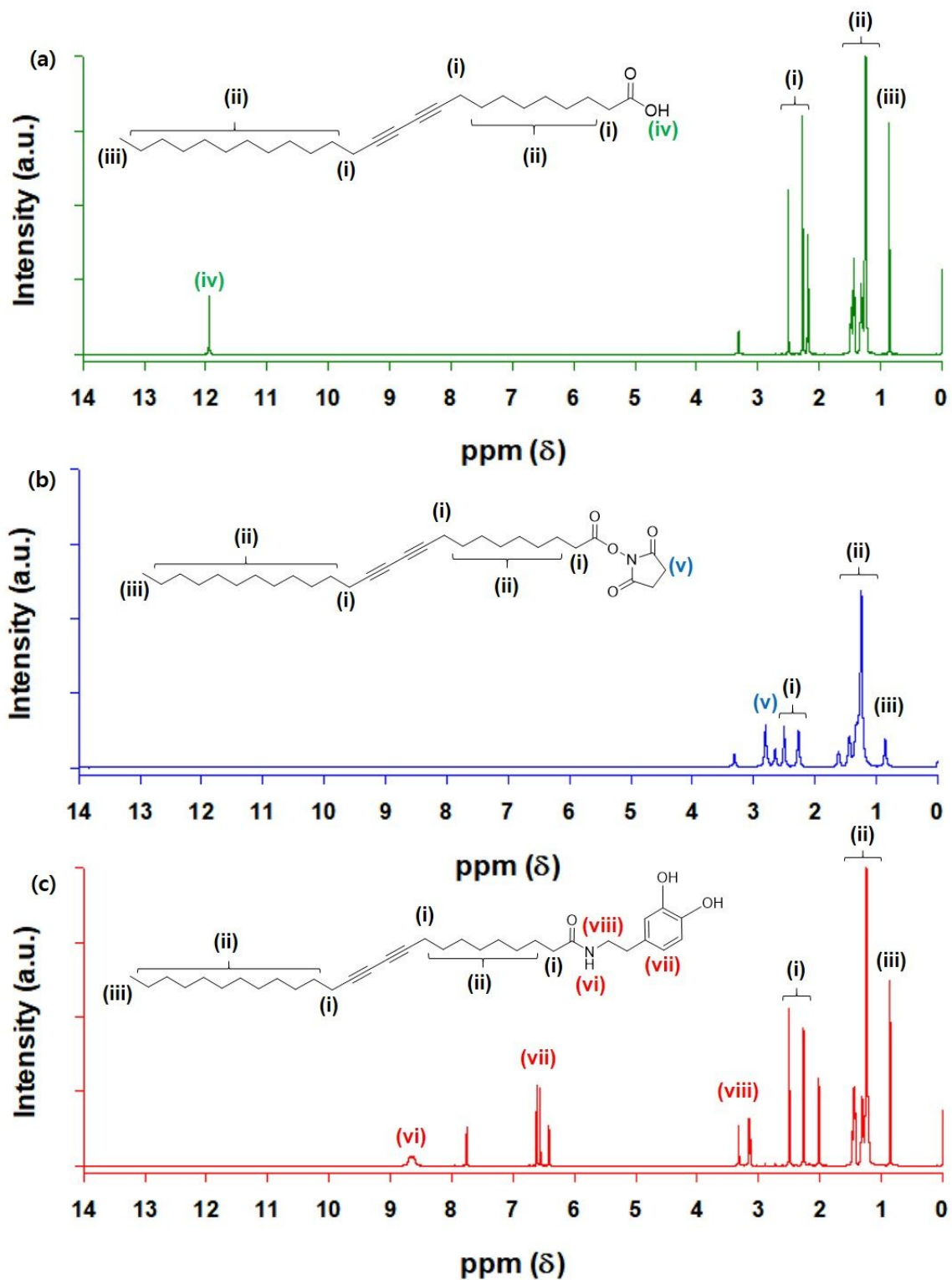


Figure S2. ¹H-NMR spectra of (a) PCDA, (b) PCDA-NHS, and (c) PCDA-Dopa.

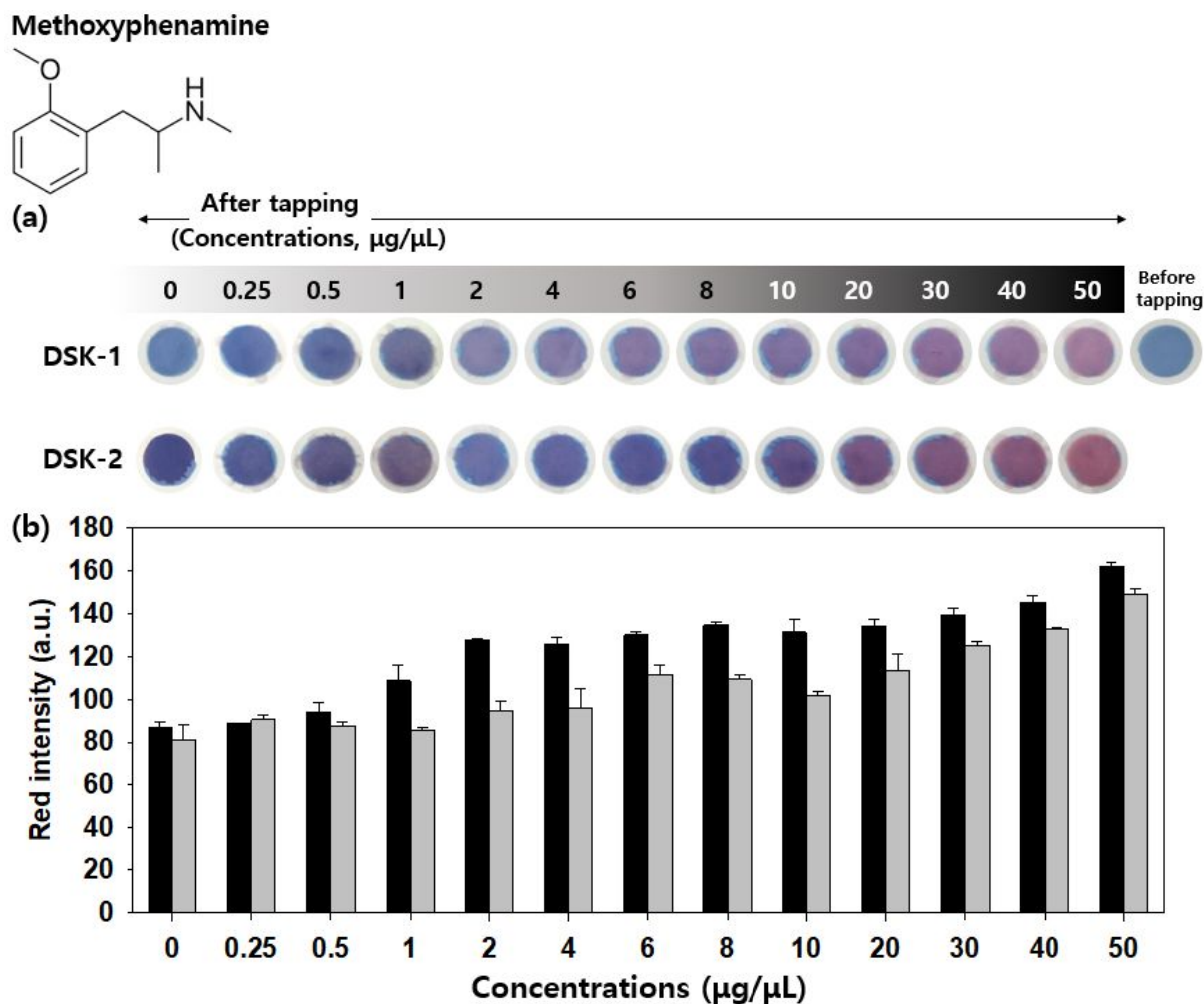
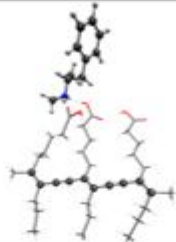
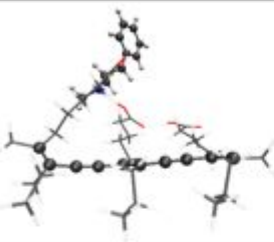
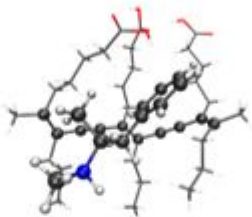



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(a) PCDA

	Top-view	Front-view	Binding energy (kcal/mol)	
Side chain			1	23.6
			2	27.7
			3	38.8
			4	34.9
			5	35.1
Backbone			6	37.5

(b) PCDA-Dopa

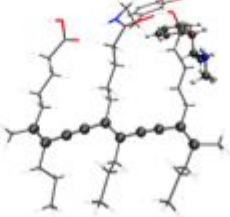
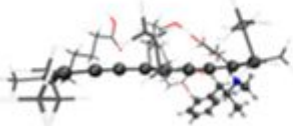


	Top-view	Front-view	Binding energy (kcal/mol)	
Side chain			1	42.8
			2	29.7
			3	31.0
			4	44.8
			5	35.4
Backbone			6	25.0

Figure S4. Quantum chemical simulations of ATSS binding to DSKs. Chemical structures of two feasible ATS binding sites in (a) PCDA trimer and (b) PCDA-Dopa trimer models. The PCDA main backbone and ATS (methamphetamine) are represented by ball-and-stick models, and the remaining atoms are represented by tube models. Binding energies of the ATS to PCDA and PCDA-Dopa depending on the binding site, side chain, and backbone.



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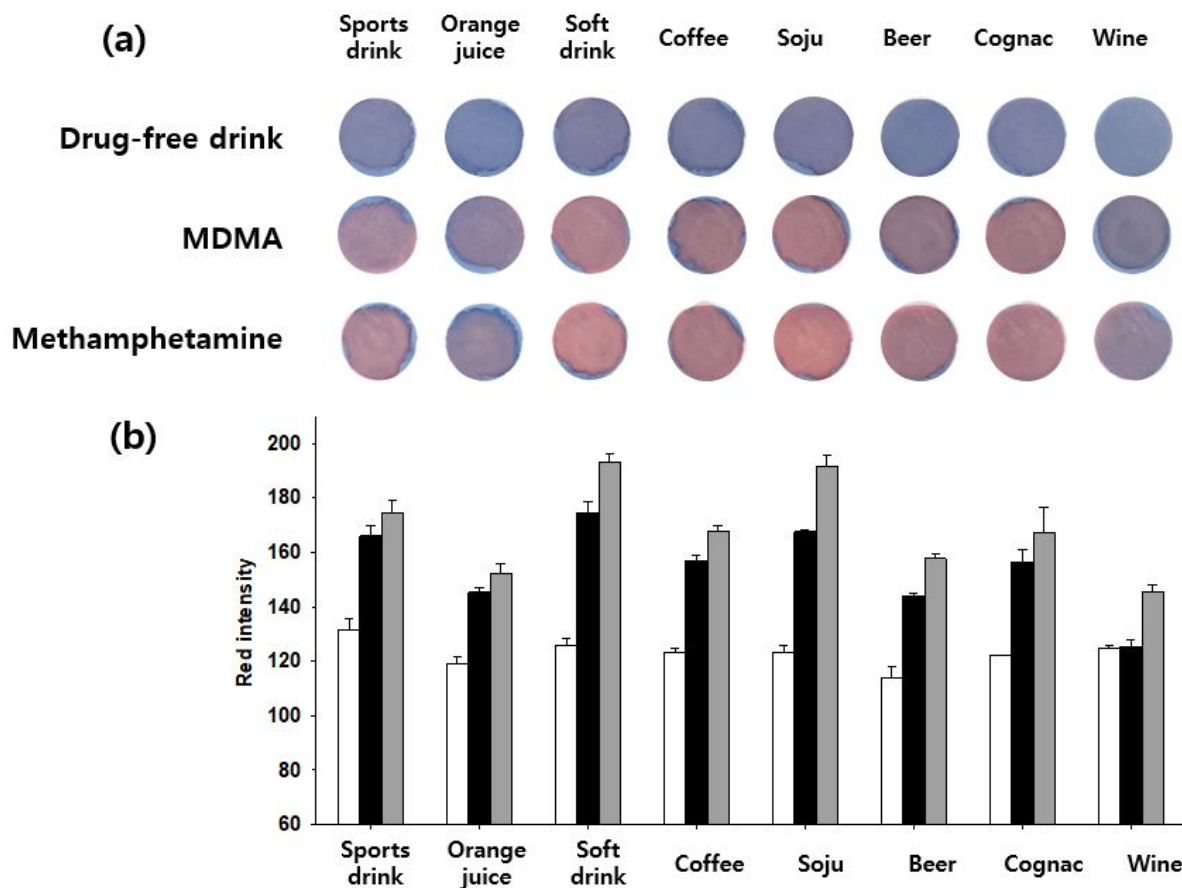


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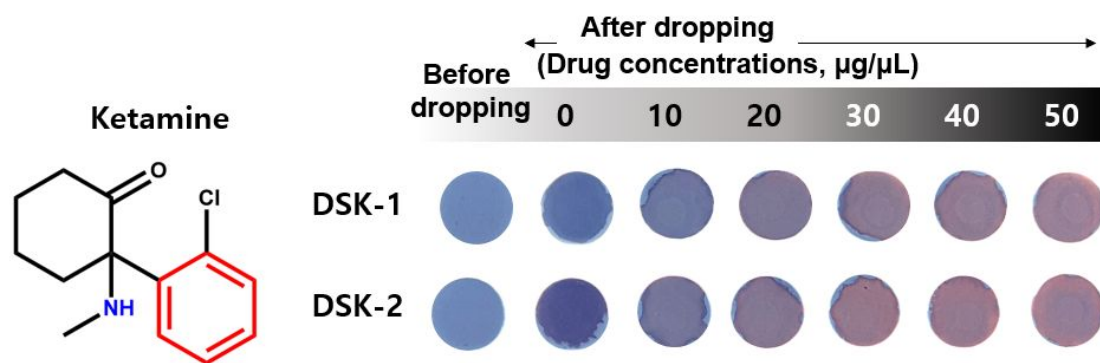


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