## Electronic Supplementary Information

for

## Evaluation of Affinity of Molecules with Carbon Nanotubes

JongTae Yoo,<sup>a</sup> Hiroaki Ozawa,<sup>a</sup> Tsuyohiko Fujigaya,<sup>a</sup>\* and Naotoshi Nakashima<sup>ab</sup>\*

<sup>a</sup>Department of Applied Chemistry, Graduate School of Engineering, Kyushu

University, 744 Motooka, Nishi-ku, Fukuoka 819-0395 Japan

<sup>b</sup>Japan Science and Technology Agency (JST), Core Research of Evolutional Science &

Technology (CREST), 5 Sanbancho, Chiyoda-ku, Tokyo 102-0075 Japan



**Fig. S1** Photograph of NMP solutions of the SWNTs before (left) and after (right) the addition of the NH<sub>2</sub>-silica.



**Fig. S2** Absorption spectra of NMP solutions of the SWNTs before (red line) and after (black line) the addition of the NH<sub>2</sub>-silica. Optical cell length:1 mm.



**Fig. S3** Chromatograms of (A) benzene, (B) naphthalene, (C) biphenyl, (D) fluorene, (E) phenanthrene, (F) anthracene, (G) pyrene, (H) triphenylene, (I) *p*-terphenyl, and (J) tetraphene obtained from  $NH_2$ -column (left) and ODS-column (right). Eluent: THF, flow rate: 0.1 mL/min.



**Fig. S4** The chromatograms of phenanthrene obtained from SWNT-column. Eluent: THF, flow rate: 0.1 mL/min. The same eluent time shows excellent reproducibility of the method.



**Fig. S5** A chromatogram of tetracene obtained from SWNT-column. Eluent: THF, flow rate: 0.5 mL/min.



**Fig. S6** Chromatograms of (a) *o*-terphenyl, (b) *m*-terphenyl, and (c) *p*-terphenyl obtained from SWNT-column ; Eluent : THF, flow rate: 0.5 mL/min.



**Fig. S7** Calculated conformations of (A) *o*-terphenyl, and (B) *m*-terphenyl on the (7,6)SWNT surface viewed from (left) the side and (right) top.







**Fig. S8** Calculated conformations of (A) benzene, (B) naphthalene, (C) biphenyl, (D) fluorene, (E) phenanthrene, (F) anthracene, (G) pyrene, (H) triphenylene, (I) *p*-terphenyl, (J) tetraphene, (K) tetracene (L) *o*-terphenyl, and (M) *m*-terphenyl on the graphene surface viewed from (left) the side and (right) top.



**Fig. S9** Chromatograms of (a) *o*-terphenyl, (b) *m*-terphenyl, and (c) *p*-terphenyl obtained from the graphite-column. Eluent: THF; flow rate: 0.1 mL/min;  $\varphi$ =1.0 mm× 30mm.