

10.1071/EN18043_AC

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Environmental Chemistry 2018, 15(5), 278-285

Supplementary Material

Binding mechanism of single-walled carbon nanotubes (SWCNTs) to serum albumin:

spectroscopy and molecular modelling exploration

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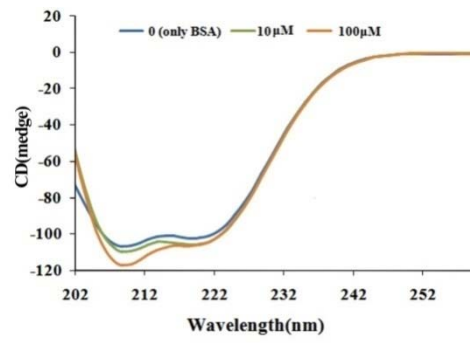


Fig. S1. Circular dichroism of BSA (10uM, pH=7.4) in the presence of different concentration of SWCNT.

Table S1. Energetic contributions of SWCNT-BSA interactions using MM-GBSA methods.

<i>Component</i>	<i>SITE I(kca/mol)</i>	<i>SITE II(kca/mol)</i>	<i>SITE III(kca/mol)</i>
ΔE_{vdws}	-15.49	-11.31	-18.11
ΔE_{ele}	-8.12	-18.59	-12.95
ΔE_{surf}	-2.82	-2.22	-3.06
ΔE_{gb}	15.17	23.68	17.80
ΔG_{gas}	-23.62	-29.90	-31.06
ΔG_{solv}	12.35	21.46	14.74
ΔG_{total}	-11.27 ± 0.68	-8.44 ± 0.48	-16.32 ± 0.98