

CBC SEMINAR ANNOUNCEMENT



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Cell Perturbation by Nanoparticles and Its Regulations

Nanomaterials are widely used in various industrial sectors, biomedicine, and more than 1300 consumer products. Although there is still no safety regulation, their potential toxicity is a major concern worldwide. We discovered that carbon nanotubes enter human cells¹, perturb cellular signaling pathways², affect various cell functions, and cause malfunctions in animals³. Because the majority of atoms in a nano-sized particle are on the surface, chemistry modification on its surface may change its biological properties significantly. To prove this hypothesis, we modified nanoparticle surface using a nano-combinatorial chemistry approach⁴. Novel nanoparticles were discovered to have a reduced toxicity, an enhanced cancer targeting ability⁵, or an increased cell differentiation regulation. Quantitative nanostructure-activity relationships (QNAR) models have been built and validated using a dataset of 84 CNTs decorated with organic surface modifiers and tested in different biocompatibility and toxicological assay. These QNAR models have been applied for virtual screening of a library collection of 240,000 ligands potentially attachable to CNT. As a proof of concept, putatively toxic and nontoxic CNTs surface-decorated by the selected ligands prioritized by QNAR model-based virtual screening were synthesized and tested. An 85% success rate was achieved. This opens new perspectives concerning the rational design of nanoparticles with controlled biological effects.

1. Mu QX, Broughton DL, Yan B. Endosomal leakage and Nuclear Translocation of Multiwalled Carbon Nanotubes: Developing a Model for Cell Uptake. *Nano Letters* 2009, 9(12), 4370-4375.
2. Mu, Q.X., Du, G.Q., Chen, T.S., Zhang, B., Yan, B. Suppression of Human Bone Morphogenetic Protein (BMP) Signaling by Carboxylated Single-Walled Carbon Nanotubes. *ACS Nano* 2009, 3, (5), 1139-1144.
3. Bai YH, Zhang Y, Zhang JP, Mu QX, Zhang WD, Butch E, Snyder S, Yan B. Repeated carbon nanotube administrations in male mice cause reversible testis damage without affecting fertility. *Nature Nanotechnology*, 2010, 5(9), 683-689.
4. Zhou, H.; Mu, Q.; Gao, N.; Liu, A.; Xing, Y.; Gao, S.; Zhang, Q.; Qu, G.; Chen, Y.; Liu, G.; Zhang, B.; Yan, B. A Nano-Combinatorial Library Strategy for the Discovery of Nanotubes with Reduced Protein-Binding, Cytotoxicity, and Immune Response, *Nano Lett.* 2008, 8 (3), 859-865.
5. Zhou, H., Jiao, P, Yang, L., Li, X., Yan, B. Enhancing Cell Recognition by Scrutinizing Cell Surfaces with a Nanoparticle Array. *J. Am. Chem. Soc.* 2010, 133(4), 680-682.

Date:	3rd July 2012 (Tuesday)
Time:	11:00am – 12:30pm
Venue:	NTU SPMS CBC Building Level 2, Conference Room
Host:	Asst Professor Liu Xuewei