Supplementary Information

Dynamic Protein Corona of Gold Nanoparticles with An Evolving Morphology

Aparna Nandakumar,^{1†} Wei Wei,^{2†} Ghizal Siddiqui,¹ Yuhuan Li,^{1,3} Aleksandr Kakinen,⁴

Xulin Wan,² Kairi Koppel,¹ Sijie Lin,⁵ Thomas P. Davis,^{1,4} David T. Leong,⁶ Darren J.

Creek,¹ Yang Song,^{7,8*} and Pu Chun Ke^{1,9*}

¹Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, 381 Royal Parade, Parkville, VIC 3052, Australia ²Key Laboratory of Luminescence Analysis and Molecular Sensing, Ministry of Education, College of Food Science, Southwest University, 2 Tiansheng Rd, Beibei District, Chongqing, 400715, China ³Liver Cancer Institute, Zhongshan Hospital, Key Laboratory of Carcinogenesis and Cancer Invasion, Ministry of Education, Fudan University, Shanghai, 200032, China ⁴Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane Qld 4072, Australia ⁵College of Environmental Science and Engineering, Biomedical Multidisciplinary Innovation Research Institute, Shanghai East Hospital, Shanghai Institute of Pollution Control and Ecological Security, Tongji University, 1239 Siping Road, Shanghai 200092, China ⁶Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117585, Singapore ⁷Key Laboratory of Luminescence Analysis and Molecular Sensing, Ministry of Education, College of Pharmaceutical Sciences, Southwest University, 2 Tiansheng Rd, Beibei District, Chongqing 400715, China ⁸State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, 100085, China ⁹The GBA National Institute for Nanotechnology Innovation, 136 Kaiyuan Avenue, Guangzhou, 510700, China

[†] These authors contributed equally.

Corresponding Authors

Email: Yang Song, yangsong@rcees.ac.cn; Pu Chun Ke, pu-chun.ke@monash.edu.



Figure S1. a) Adsorption measurement at 562 nm for different AuNP protein coronae. b) Total amount of proteins bound to different AuNPs (1 mg), determined from the BCA protein assay interpolating the BSA standard.



-1 -2





Figure S2. Hierarchical clustering heatmap for all 275 coronal proteins identified across the three AuNP groups.



Figure S3. Volcano plot for the fold-change analysis (coronal proteins with a fold change cutoff below 0.5 and above 1.5, and with a *P*-value < 0.05) of a) AuNP₁ vs. AuNP₂ and b) AuNP₂ vs. AuNP₃.



Figure S4. Coronal protein enrichment represented by a) grand average of hydropathy (GRAVY) index, b) isoelectric point (pI), and c) molecular weight for the common proteins identified across the AuNP series.



Figure S5. Compiled protein network for all 173 StringDB identified coronal proteins (out of 275, immunoglobulin sidechains excluded) across the three types of AuNPs.



Figure S6. Protein interactive network generated in Cytoscape for the differentially associated coronal proteins on AuNP₁&AuNP₃. The relative fold change abundance (AuNP₁/AuNP₃) is indicated by the motif color and the size indicates the *p*-value for the relative fold change data. Cluster maker app from the cytoscape using Markov CLustering Algorithm (MCL) was used to highlight the enrichment of Apolipoproteins and other proteins involved in the cholesterol metabolism pathways in spiky AuNP₁.



Figure S7. Mean intensity comparison of top-10 abundant immunoglobulin sidechains associated with the coronal proteins of the three types of AuNPs.