

Supplementary Material for

Title: Nanotube abundances from non-negative matrix factorization of Raman spectra as an example of chemical purity from open source machine learning

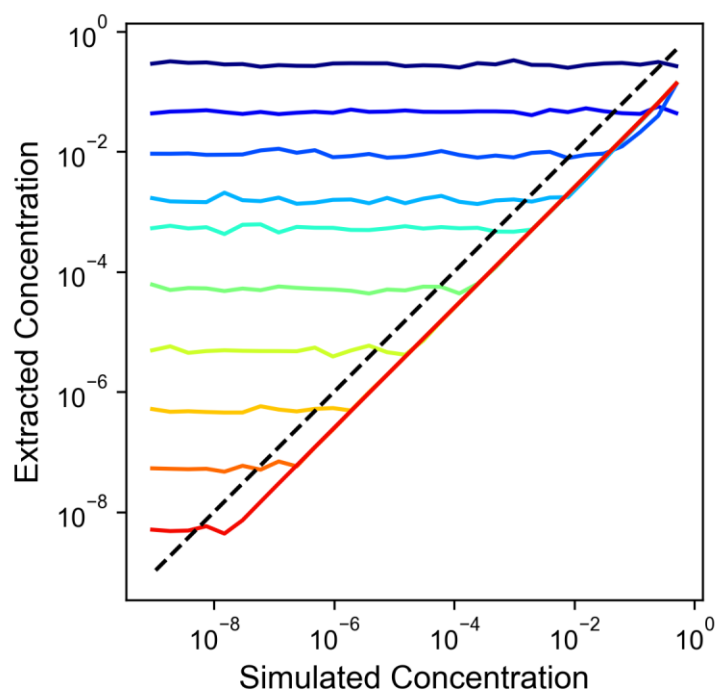
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**Figure S1 Extracted Concentration vs. Simulated Concentration**

This is the same as Figure 2(e), but plotted in concentration. (See main text).

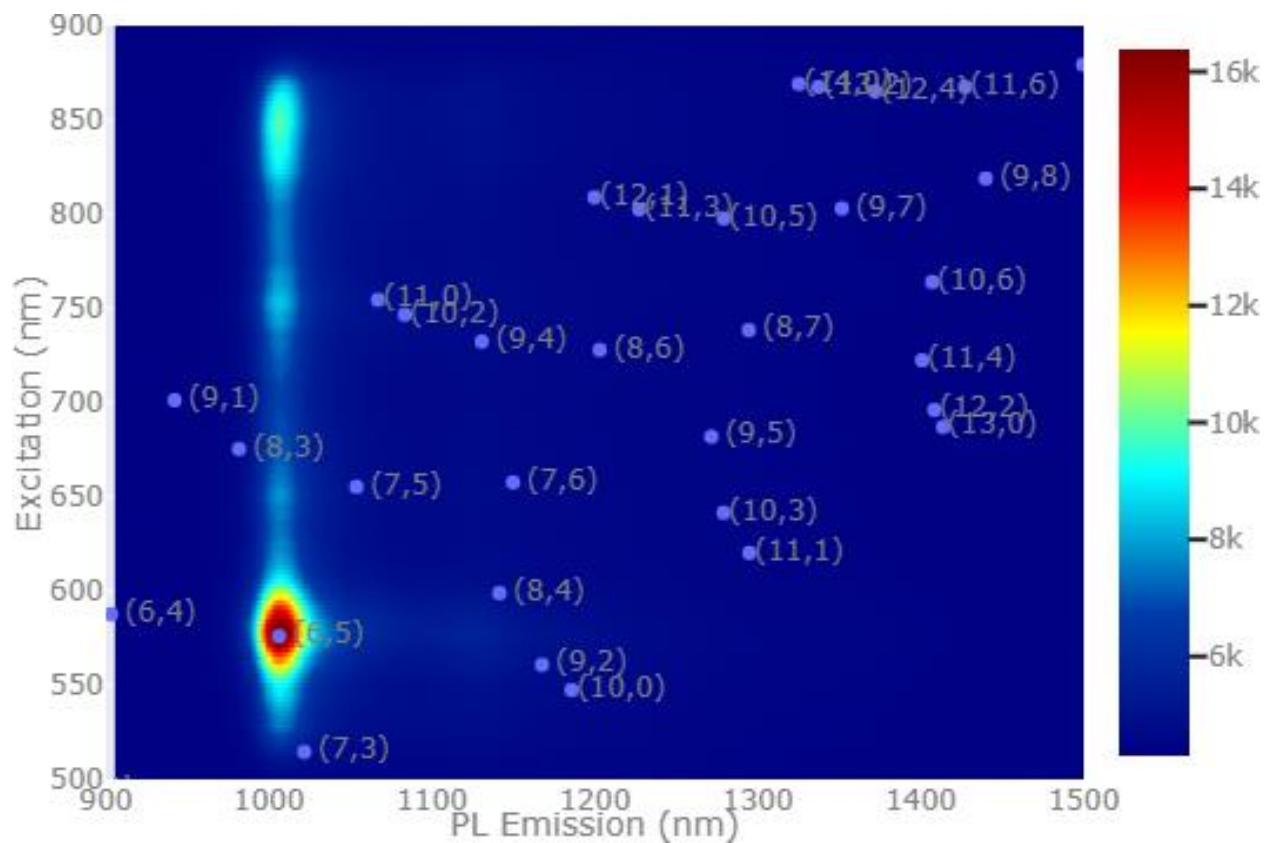
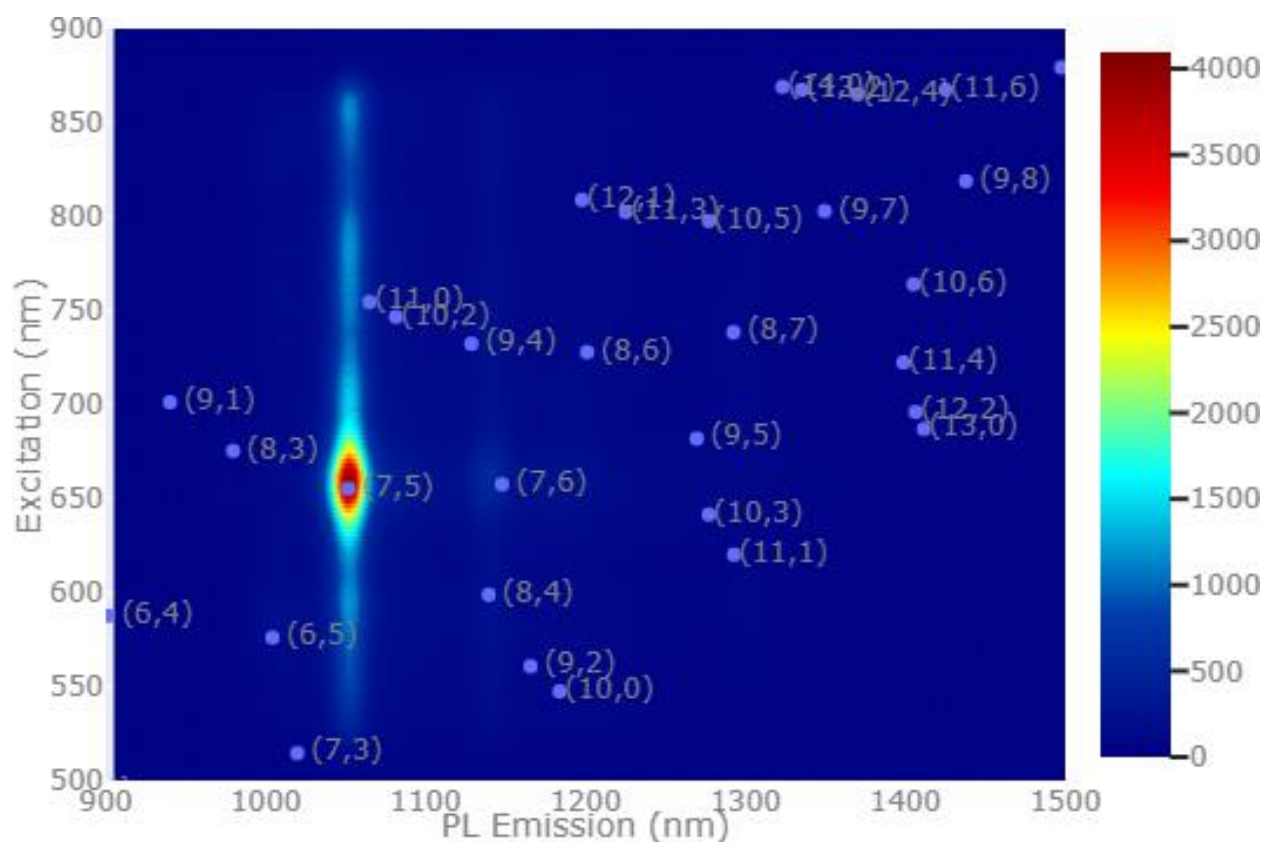


Figure S2 Photoluminescence Excitation Map of (6,5) SWNCT Stock Liquid



**Figure S2 Photoluminescence Excitation Map of (7,5) SWNCT Stock Liquid**

The photoluminescence excitation maps are taken with a real-time supercontinuum system after ref. [s1]. Positions of the  $(n,m)$  peaks are derived from ref [s2], allowing for a small dielectric shift due to the different environment, after ref. [s3]

[s1] J. Lefebvre, ACS Nano (2016) 9602

[s2] R. B. Weisman, S. M. Bachilo, Nano Letters(2003) 1235

[s3] J. Lefebvre, J. Fraser, Y. Homma, P. Finnie, Appl. Phys. A (2004) 1107