

SUPPLEMENTARY MATERIAL FOR:

**Classification of the Lung Cancer Histology by Gold
Nanoparticle Sensors**

Orna Barash^{1,⊥}, Nir Peled^{2,3,⊥}, Ulrike Tisch¹, Paul A. Bunn Jr. R.², Fred R. Hirsch², and
Hossam Haick^{*1}

[⊥] *The two authors have contributed equally to this work.*

¹ *The Department of Chemical Engineering and Russell Berrie Nanotechnology Institute, Technion – Israel Institute of Technology, Haifa 32000, Israel.*

² *University of Colorado Cancer Center, Division of Medical Oncology, UC Denver, Aurora, Colorado 80045, US*

³ *The Lung Cancer Unit, Sheba Medical Center, Tel Aviv University, Tel Aviv 52621, Israel.*

Table S1: Organic ligands and baseline resistance of the 18 GNP chemiresistors that were simultaneously exposed to the headspace samples. Four sensors were selected via SVM analysis for the listed applications, based on their discriminative power.

Sensor	Organic Ligand	Baseline resistance (MΩ)	Application(s)
1	Decanethiol	6.3	LC* - IBE [†] ; SCLC [‡] – NSCLC [§] ; and Adenocarcinoma – Squamous cell carcinoma
2	Hexanethiol	3	SCLC – NSCLC; and Adenocarcinoma – Squamous cell carcinoma
3	Butanethiol	1	SCLC – NSCLC; and
4	2-Mercaptobenzoxazole	1	Adenocarcinoma – Squamous cell carcinoma
5	Dodecanethiol	13	Not used for this study
6	4-Methoxy-toluenethiol	3	
7	11-Mercapto-1-undecanol	4.7	
8	Octadecanethiol	24	
9	4-trifluoromethyl-benzenethiol	0.6	
10	2-Ethylhexanethiol	9	
11	3-Methyl-1-butanethiol	10	
12	3-Methyl-1-butanethiol & hexanethiol	0.3	
13	2-Mercaptobenzylalcohol	0.1	
14	11-Mercapto-1-undecanol	12	
15	Tert-dodecanethiol	2	
16	3-Mercapto-propionate	0.4	
17	Dibutyl disulfide	0.6	
18	3-Methyl-1-butanethiol & dodecanethiol	0.2	

* LC: Lung cancer

† IBE: Immortal bronchial epithelium

‡ SCLC: Small cell lung cancer

§ NSCLC: Non-small-cell-lung cancer

Table S2: The number of correct and incorrect sample classifications, estimated by supportive vector machine (SVM) and cross-validation of medium 1 and of medium 2. The input features for the SVM analysis were the same as for the distinction between LC and IBE (three features from sensor 1, *see* Figure 1(a)), and the same correction was applied. The two growth mediums could not be distinguished, showing that the LC-IBE distinction does not stem from the use of the different growth mediums.

	Classified as Medium 1	Classified as Medium 2
Medium 1 (all LC cell lines)*	4	3
Medium 2 (IBE cell lines)*	4	1

* The sensing features were corrected by subtracting the mean value of the corresponding medium.

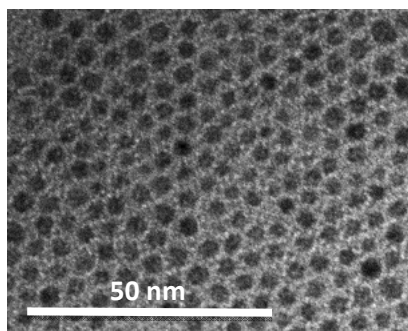


Figure S1: Representative transmission electron micrograph (TEM) of the decanethiol-functionalized GNPs (sensor 1) in solution, which formed a continuous film connecting the microscopic interdigitated circular gold electrodes (*see* inset of Figure 1C), providing multiple conductive pathways between them.

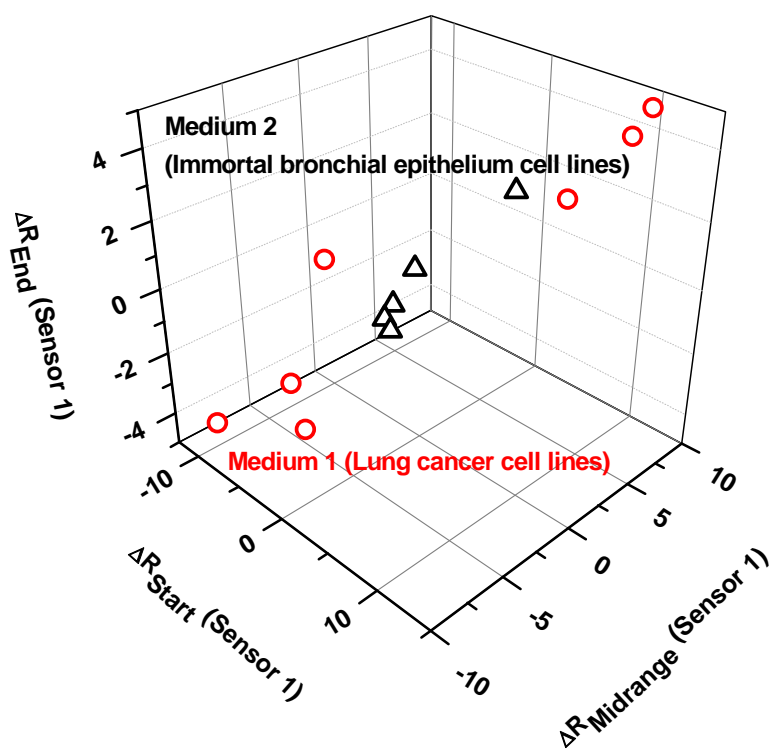


Figure S2: Corrected sensing features for the headspace samples that were collected from medium, which was used to grow all the lung cancer (LC) cell lines (7 replicas), and of medium 2, which was used to grow all the immortal bronchial epithelium (IBE) cell lines (5 replicas). Total overlap of the sensing features was observed and SVM analysis could not distinguish between the two mediums (*see* Supporting Table S2).