

## End-Selective Functionalization of Carbon Nanotubes. Use of DOE for the Optimization of a DNA Probe Attachment and Hybridization Using an Enzymatic Amplifying System

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### Electronic Supplementary Information (ESI)

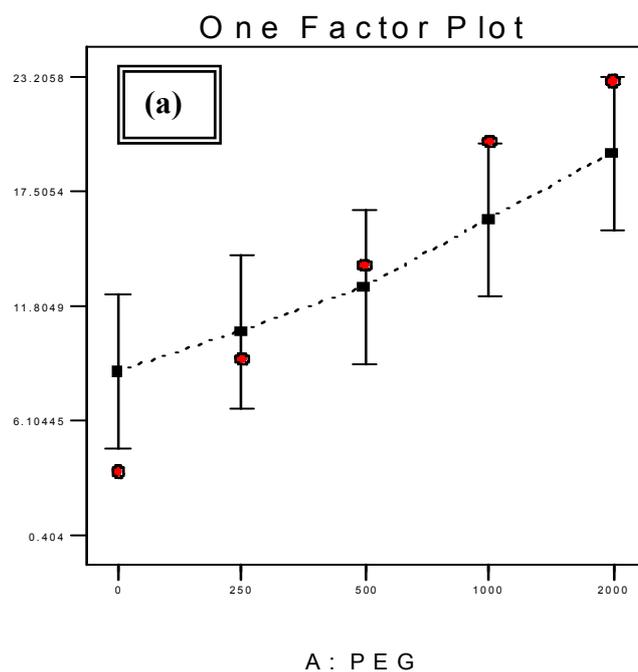
Category Protocol N°	Total Binding (OD)	Non-Specific Binding (OD)	EF (n° 1) <sup>a</sup>	Pegylated MWCNT <sub>s<sub>ox</sub></sub> : Total Binding (OD)	Pegylated MWCNT <sub>s<sub>ox</sub></sub> : Non-Specific Binding (OD)	EF (n° 2) <sup>b</sup>
8	2.22	1.06	1.1	1.04	0.03	32.8
7	2.11	1.30	0.6	1.20	0.03	48.0
3	2.82	1.25	1.3	0.51	0.05	9.5
5	2.53	1.25	1.0	1.09	0.04	27.5
1	2.68	1.43	0.9	1.25	0.03	37.0
2	2.92	1.24	1.4	1.18	0.03	36.9
6	1.44	1.19	0.2	1.04	0.03	33.0
4	1.80	1.28	0.4	1.04	0.03	33.0
Stand. 9	3.30	2.38	0.4	1.33	0.04	34.1

Table ESI-1. OD and EF data for the 1<sup>st</sup> randomly executed set of DOE experiments involving *non-pegylated (a, n° 1)* and *pegylated (b, n° 2)* oxidized MWCNT<sub>s<sub>ox</sub></sub>

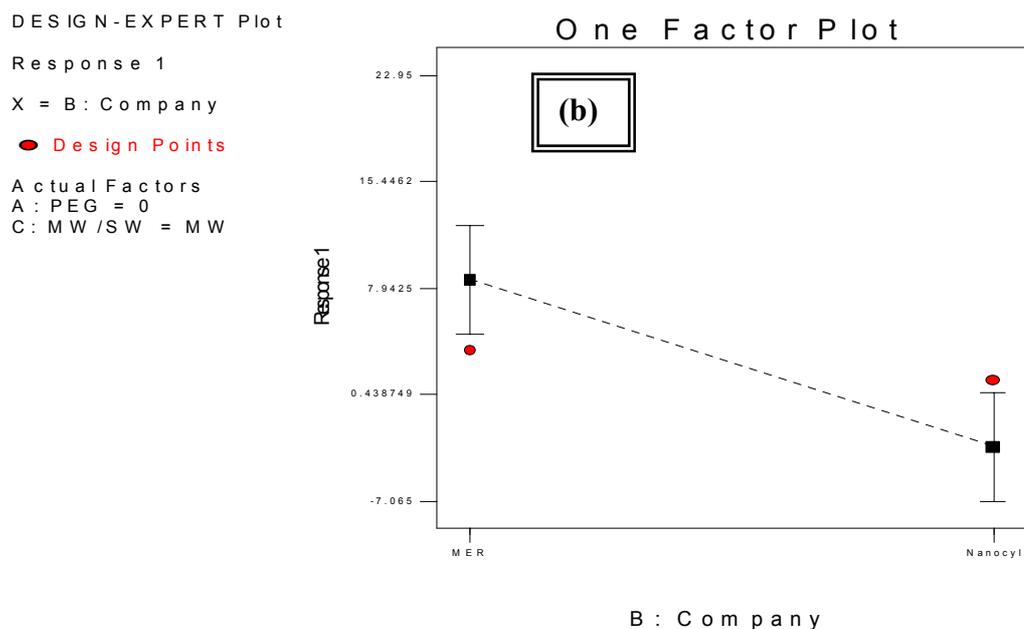
DESIGN-EXPERT Plot

Response 1  
X = A : PEG  
● Design Points  
Actual Factors  
B : Company = MER  
C : MW / SW = MW

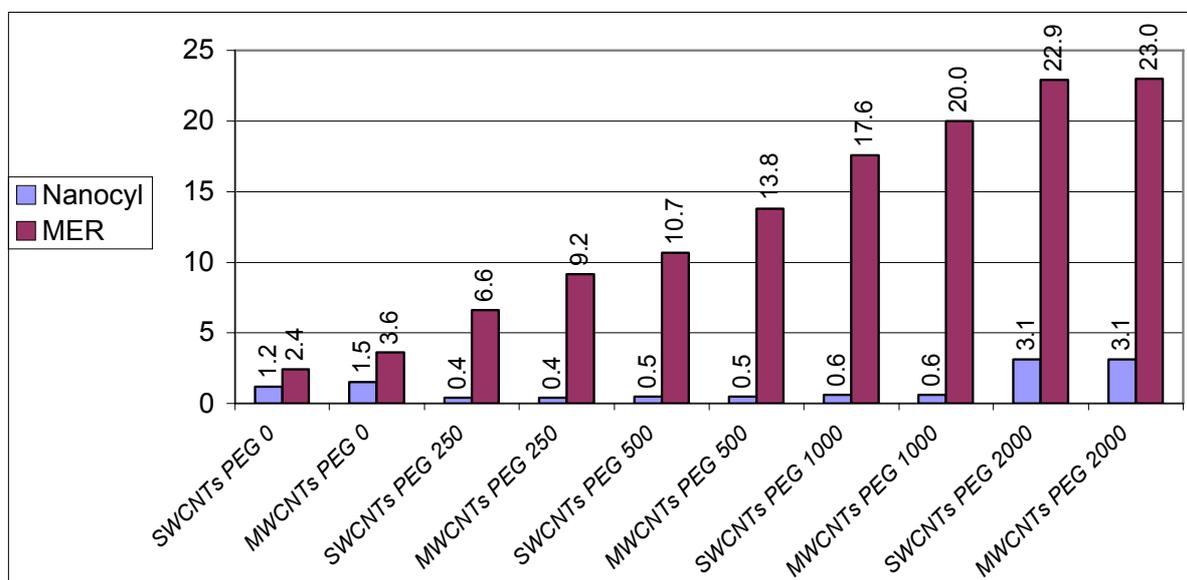
1  
e  
s  
n  
R  
p  
s  
e  
R



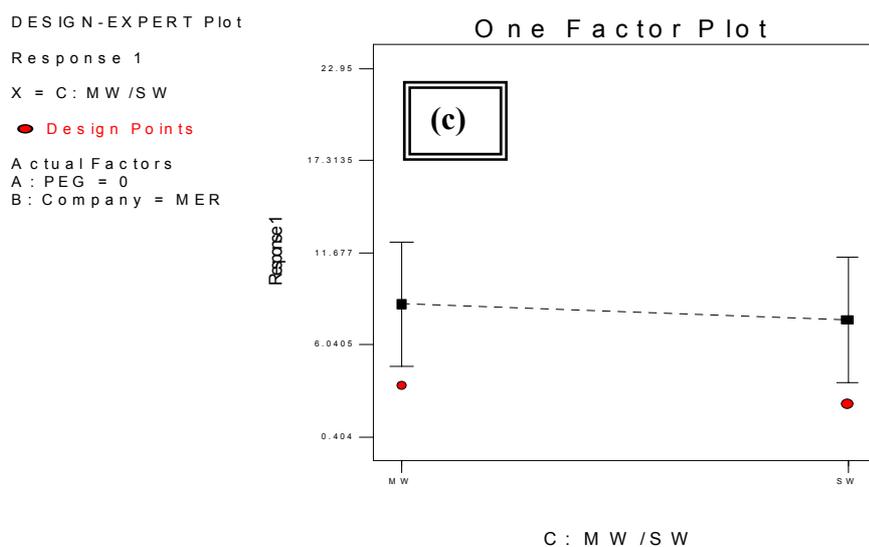
**Figure ESI-1a (One Factor Plot Graph).** Optimal conditions for the oxidative opening of MWCNTs and sidewall PEG-mediated passivation from DOE experiments (influence of the molecular weight of the PEG polymer)



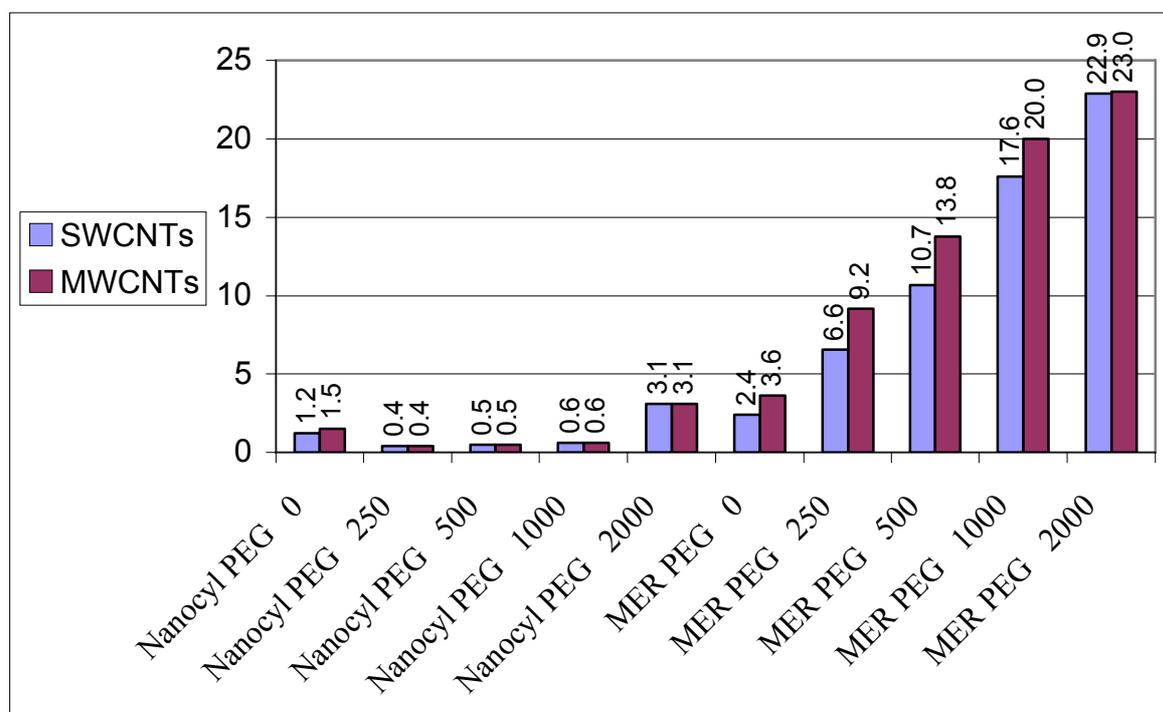
**Figure ESI-2a (One Factor Plot Graph).** Optimal conditions for the oxidative opening of MWCNTs and sidewall PEG-mediated passivation from DOE experiments (influence of the commercial source of MWCNTs/SWCNTs)



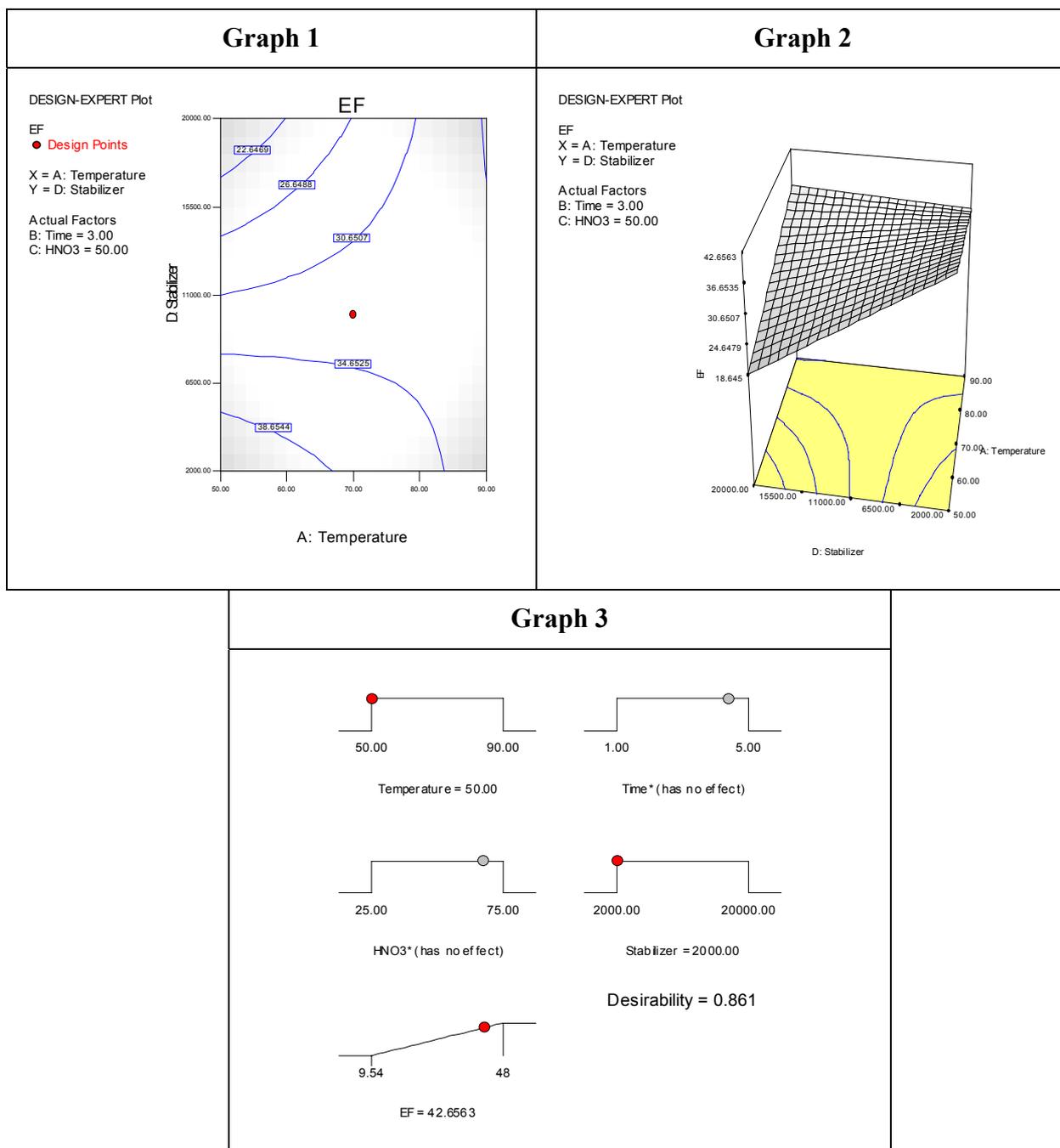
**Figure ESI-2b.** Influence of the commercial source of MWCNTs/SWCNTs (MER Corporation Ltd. and Nanocyl s.a.)



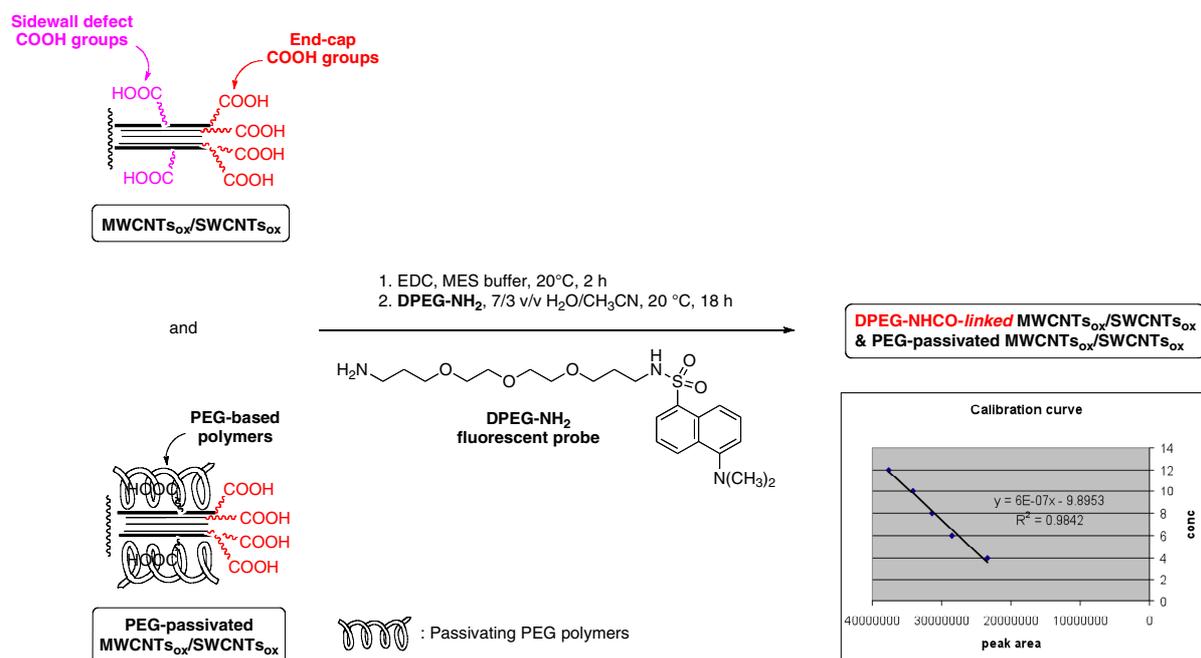
**Figure ESI-3a (One Factor Plot Graph).** Optimal conditions for the oxidative opening of MWCNTs and sidewall PEG-mediated passivation from DOE experiments (influence of the *multi-* or *single*-walled type of starting MWCNTs/SWCNTs)



**Figure ESI-3b.** Influence of the *multi-* or *single*-walled type of starting MWCNTs/SWCNTs



**Figure ESI-4. Graphs 1-3:** Sequence optimization and optimal conditions disclosed from a 1<sup>st</sup> set of DOE experiments using an HRP-amplifying DNA-based hybridization system



**Scheme ESI-1.** Quantification of accessible end- versus sidewall-localized COOH groups using the EDC-mediated covalent attachment of the fluorescent probe **DPEG-NH<sub>2</sub>**