Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information for

Quantification of Multiwall Carbon Nanotubes in Plant Tissues with Spectroscopic Analysis

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Calculation of detection limit. Based on the regression in Figure 4,

$$ABS_{obs} - ABS_{BK} = k * C_{CNT} + b$$

Where ABS_{obs} is the observed absorbance at 800 nm, ABS_{BK} is the background absorbance value of leaf/stem/root, C_{CNT} is the concentration of CNT (μg/g), k is the coefficient for $C_{CNT,}$ b is the regression constant. The detection limit for C_{CNT} was determined, when the difference between ABS_{obs} and ABS_{BK} equals to three times the standard deviation for $ABS_{BK.}$ The corresponding values and detection limit for p/c-MWCNT in leaf/stem/root were listed in Table S4.

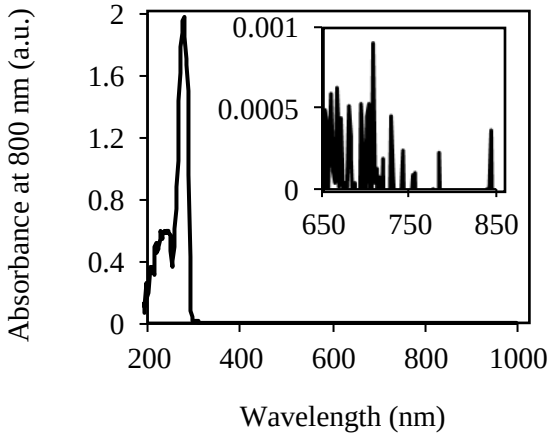

Figure S1: UV-Vis spectra of TX-100 (2.0 mg/mL) at 200-1000 nm. The peak was obtained at 276 nm, followed by a flat line reached at baseline after 300 nm.

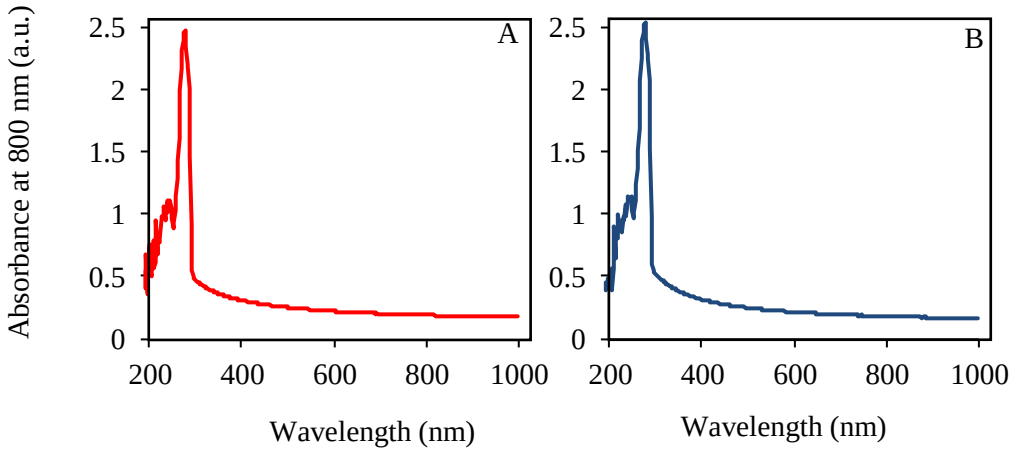

Figure S2: UV-Vis spectra of p-MWCNTs (A) and c-MWCNTs suspended with TX-100 (2.0 mg/mL) at 200-1000 nm. The peak was obtained at 276 nm from the TX-100, followed by featureless spectra at 300-900 nm.

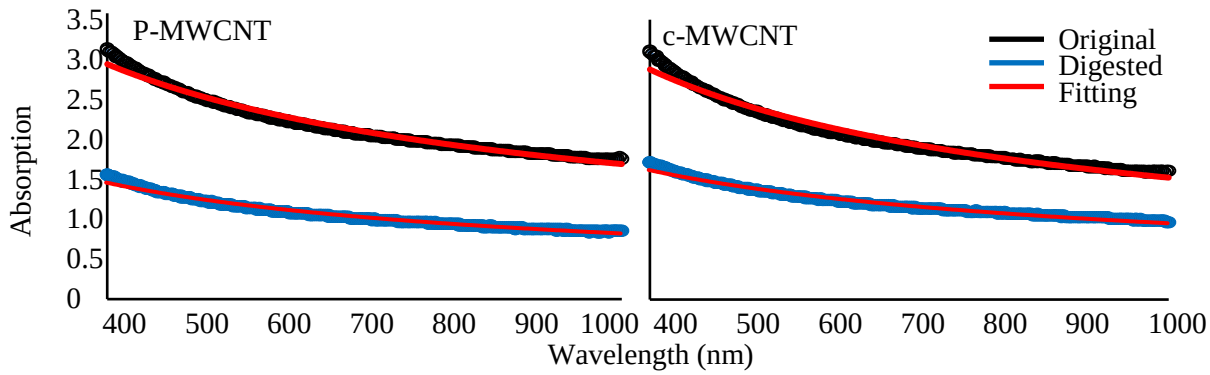

Figure S3: Power-law regression for wavelength-dependent absorption of MWCNTs

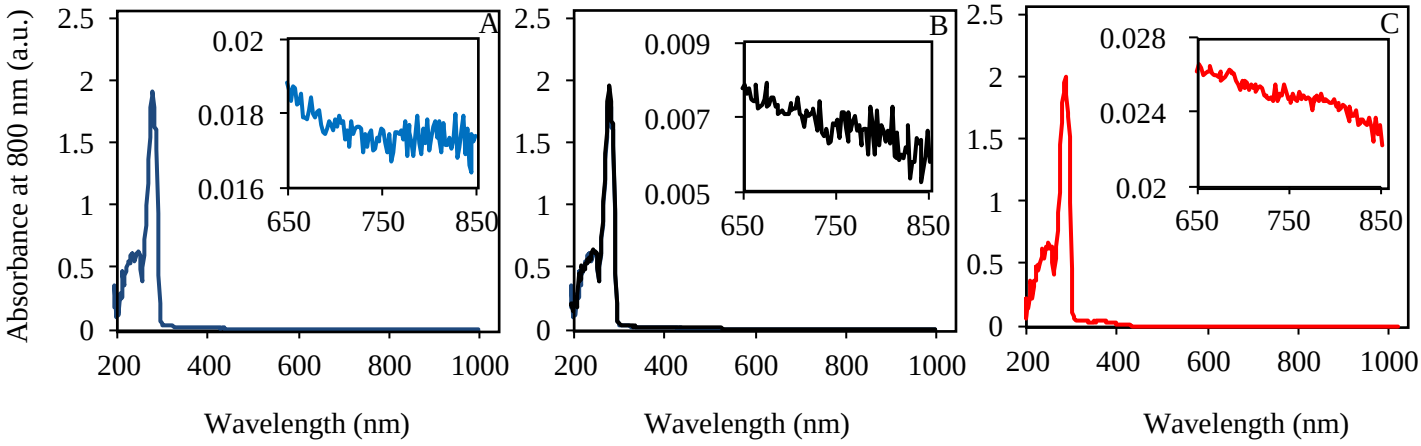

Figure S4: UV-Vis spectra of digested leaf and stem, and suspended with TX-100 (2.0 mg/mL) at 200-1000 nm. The peak was obtained at 276 nm for TX-100, followed by a flat line reached at baseline after 300 nm. The area at 650-850 is zoomed and shown in the box.

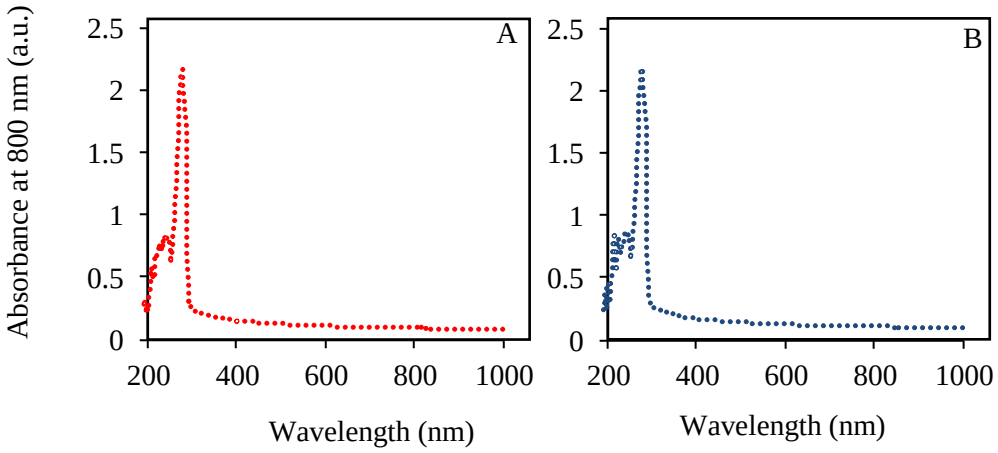

Figure S5: UV-Vis spectra of p-MWCNTs (A) and c-MWCNTs (B) at 200-1000 nm after digestion and suspended with TX-100 (2.0 mg/mL). The peak was obtained at 276 nm from the TX-100, followed by featureless spectra at 300-900 nm.

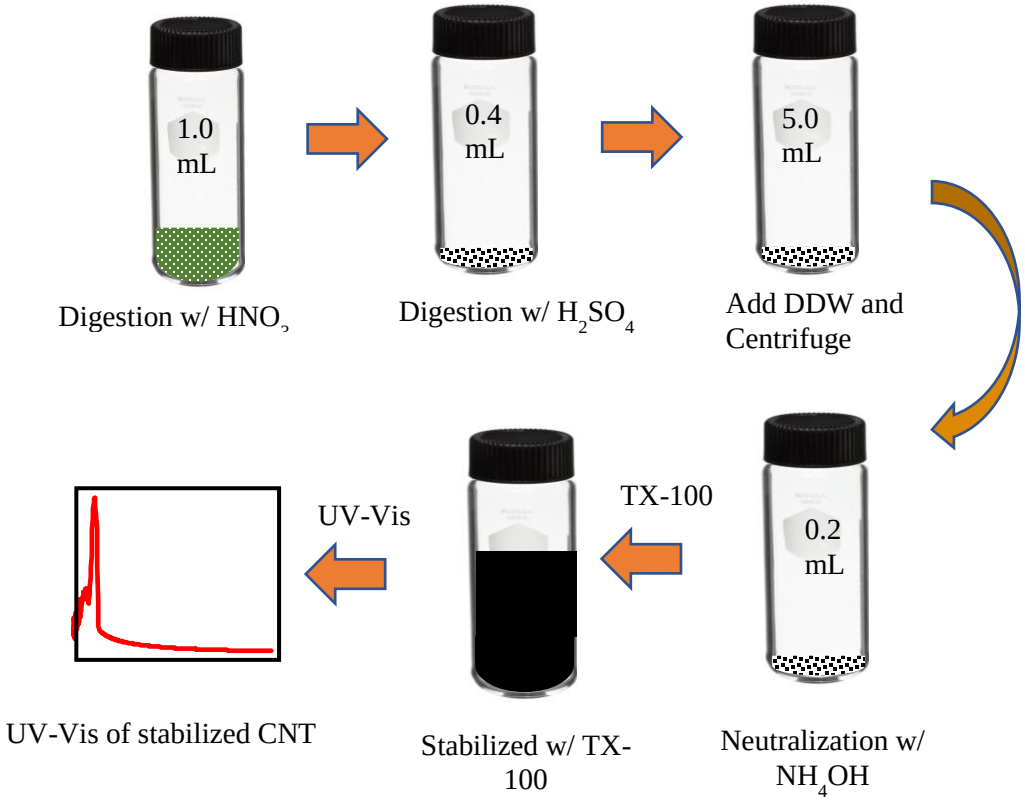

Figure S6: The final digestion scheme for sample preparation for spectroscopic analysis.

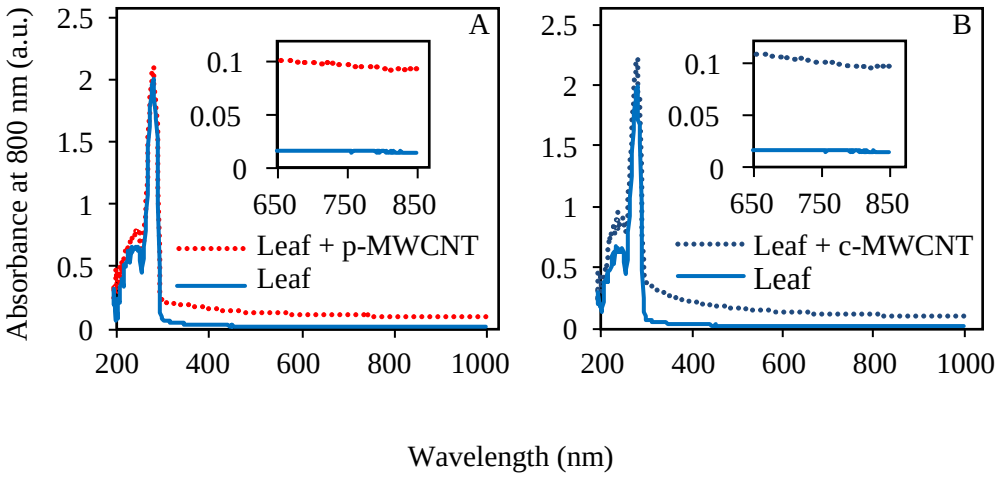

Figure S7: The spectra for p-MWCNTs (A), or c-MWCNTs (B) spiked leaf tissues digested, and suspended with TX-100. The panel inside shows the area zoomed at 650-850 nm.

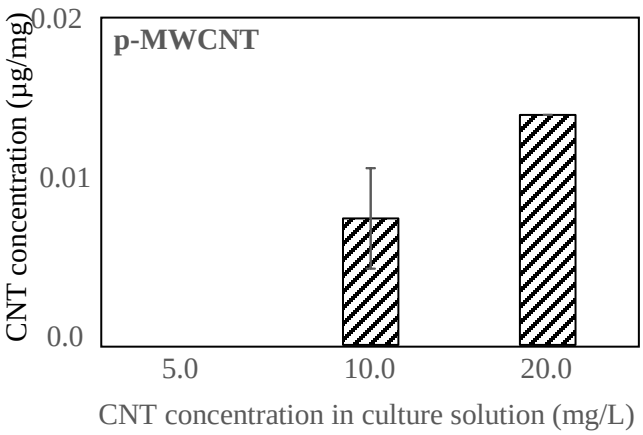

Figure S8: Concentrations of p-MWCNT in lettuce leaves quantified by digestion coupled with analysis of UV-Vis absorbance at 800 nm. The plants were grown in greenhouse at hydroponic system containing 5, 10, and 20 mg/L CNT solutions.

Table S1 Major physicochemical properties of CNTs used in this study.

Properties	p-MWCNT	c-MWCNT	Characterization methods
Average length (μm)	<1.0	<1.0	TEM (from the manufacturer)
Average diameter (nm)	9.5	9.5	TEM (from the manufacturer)
Bulk carbon content (%)	97%	85.9%	Elemental analysis
Bulk carboxyl	NA	<8%	TGA (from the manufacturer)
COOH (surface)	1.2%	1.95%	XPS
C=O (surface)	4.28%	5.07%	XPS
C-O (Surface)	7.71%	9.62%	XPS

Table S2. Regression equation and statistics for p-MWCNT in Figure 4. Y indicates the detected UV-Vis absorbance at 800 nm calibrated by the background, and x indicates the applied p-MWCNT concentration in digestion solution (μg/mL) or lettuce tissues (μg/mg).

Sample	x	Equation	R^2	P-value
p-MWCNT + Leaf	concentration in digestion solution (μg/mL)	y = 0.0097x - 0.000050	0.99	<0.01
p-MWCNT + Leaf	concentration in leaf tissues (μg/mg)	y = 0.20x - 0.00060	0.99	<0.01
p-MWCNT + Stem	concentration in digestion solution (μg/mL)	y = 0.0066x - 0.003	0.99	<0.01
p-MWCNT + Stem	concentration in stem tissues (μg/mg)	y = 0.14x - 0.0054	0.99	<0.01
p-MWCNT + Root	concentration in digestion solution (μg/mL)	y = 0.0086x + 0.0081	0.95	<0.01
p-MWCNT + Root	concentration in root tissues (μg/mg)	y = 0.16x + 0.015	0.95	<0.01

Table S3. Regression equation and statistics for c-MWCNT in Figure 4. Y indicates the detected UV-Vis absorbance at 800 nm calibrated by the background, and x indicates the applied c-MWCNT concentration in digestion solution (μg/mL) or lettuce tissues (μg/mg).

Sample	x	Equation	R^2	P-value
c-MWCNT + Leaf	concentration in digestion solution (μg/mL)	y = 0.0064x + 0.0062	0.98	<0.01
c-MWCNT + Leaf	concentration in leaf tissues (μg/mg)	y = 0.12x + 0.012	0.98	<0.01
c-MWCNT + Stem	concentration in digestion solution (μg/mL)	y = 0.0098x - 0.0044	0.97	<0.01
c-MWCNT + Stem	concentration in stem tissues (μg/mg)	y = 0.20x - 0.0079	0.97	<0.01
c-MWCNT + Root	concentration in digestion solution (μg/mL)	y = 0.0076x - 0.0059	0.94	<0.01
c-MWCNT + Root	concentration in root tissues (μg/mg)	y = 0.17x - 0.013	0.94	<0.01

Table S4. Key parameters used for calculation of detection limit by using UV-Vis absorbance at 800 nm.

		Background	Standard deviation	*k*	*b*	Detection limit (μg/mg)
p-MWCNT	Leaf	0.022	0.008	0.2	-0.0006	1.23E-01
	Stem	0.008	0.002	0.14	-0.0054	8.14E-02
	Root	0.015	0.006	0.16	0.015	1.88E-02
c-MWCNT	Leaf	0.022	0.008	0.12	0.012	1.00E-01
	Stem	0.008	0.002	0.2	-0.0079	6.95E-02
	Root	0.015	0.006	0.17	-0.013	1.82E-01