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***Environmental Science: Nano* Supporting Information**

Proteomic, gene and metabolite characterization reveal uptake and toxicity mechanism of cadmium sulfide quantum dots in soybean plants

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The following Supporting Information is available for this article:

Supporting Methods

Supporting Tables (* due to the large volume of some tables, the marked ones are included in a separate supporting excel document)

Supporting Figures

Fig. S2. Multi-scatter plots of the identified proteins (including Pearson's coefficient) in the soybean roots exposed to ION, BULK and CdS-QDs.

Method S1. Sample preparation for proteomic analysis

The frozen ground soybean root tissues (~60 mg each) were solubilized in 600 µl extraction buffer containing 50 mM Tris-HCl (pH 8.8), 5 mM dithiothreitol (DTT), 1 mM ethylenediaminetetraacetic acid, 1% (v/v) Triton X-100, and 1% (v/v) Plant Protease Inhibition Cocktail (Sigma, MO, USA). The samples were then subjected to 20 min vortexing, 20 min bath sonication, and 20 min centrifugation at 14,000 g. A temperature of 4 °C was maintained throughout the extraction process. Proteins in the supernatants were precipitated overnight at -20 °C using 4 volumes of 10 % trichloroacetic acid in acetone, containing 20 mM DTT. The protein pellets were obtained by centrifugation at 14,000 g and were washed successively with acetone three times and solubilized in 100 µl of 50mM ammonium bicarbonate containing 8M urea. The protein (~20 µg) in the samples was reduced and alkylated, followed by overnight digestion at 37 °C using MS grade trypsin (Thermo Scientific Pierce Trypsin Protease) at an enzyme: substrate ratio of 1:20 (w/w). Digestion was stopped using formic acid (FA) to a final concentration of 5% in solution. The peptide in solutions were then desalted using Pierce C-18 StageTips, eluted in 40% ACN, dried and resuspended in 5% FA prior to liquid chromatography- tandem mass spectrometry (LC-MS/MS) analysis using a Thermo Easy-nLC system coupled to a Thermo Q-Exactive mass spectrometer.

Each sample (4 µl) was injected in a sequence into a C18 reversed phase (3 uM, 100A pores, Dr. Maisch GmbH) column, packed in-house with 100uM ID and 18cm resin. Digested peptides were eluted on a 140 min water-acetonitrile gradient at a flow rate of 300 nL/min, with 3% DMSO in both buffers under electrospray ionization of 2.2kV. The MS/MS spectra was generated by data-dependent spectral acquisition strategy in the mass spectrometer consisting of a repeating cycle of one full MS spectrum at a resolution of 70,000 (mass range 400-1800 m/z and AGC target value of 1.0E6) in the Orbitrap analyzer, followed by MS/MS of precursor ions from the full MS scan by higher-energy collisional dissociation (HCD) with a fixed injection time of 120 ms, resolution of 17,500 and AGC target value of 5.0E4.

Method S2. Targeted analysis of metabolite groups

LC-MS/MS analysis of metabolites. Frozen tissues (~80 mg) were extracted in 1 ml of 80% methanol in LC-MS-grade water containing 2% formic acid by consecutive vortexing and sonication in water bath for 30 min each. The extracts were centrifuged for 30 min at 20,000 ×g and the

supernatants were used for detection and quantification of 46 plant metabolites including organic acids, amino acids, and antioxidants using Agilent 1260 UHPLC binary pump coupled with Agilent 6470 triple quadrupole mass spectrometer, using external standard calibration for organic acids and antioxidants, and isotopically labelled internal standard calibration for amino acids. A set of 22 amino acids and 12 antioxidants in the plant tissues were separated via Agilent InfinityLab Poroshell 120 HILIC-Z (2.1 × 100 mm, 2.7 μm) and Agilent ZORBAX StableBond 80 Å C18 (4.6 mm × 50 mm, 3.5 μm) columns, respectively, and were analyzed following previous methods with minor adjustments (1, 2). Organic acids were separated on an Agilent Polaris C-18-Ether (150 x 3.0 mm) column using water and methanol containing 0.1% formic acid as mobile phases. Twelve organic acids were separated within 8 min after injecting 2 μL onto the column following an increasing gradient of methanol phase from 25 % at 0 min to 60 % at 1 and 8 min. MS spectra for the organic acids were acquired using spray ionization at 2,500 V in negative mode.

Method S3. Real time qPCR analysis of targeted genes

Total RNA was extracted from 0.1 g of ground root and shoot tissues using a Sigma Aldrich Spectrum Plant Total RNA Kit (Sigma Aldrich, St. Louis, MO, USA). A NanoDrop Lite Spectrophotometer (Thermo Fisher Scientific, Wilmington, DE) and gel electrophoresis was used to assess the RNA quality and quantity. Reverse transcription was performed on 1 μg of the total extracted RNA using the Qiagen QuantiTect Reverse Transcription kit (Qiagen, Velno, Netherlands). qPCR amplifications were carried out using Bio-Rad SsoAdvanced™ Universal SYBR® Green Supermix (Bio-Rad, Hercules, CA, USA) in an optical 96-well plate with a Bio-Rad CFX96 Touch™ Real-Time PCR Detection System. Gene sequences were obtained through the BLAST tool of PlantGDB (www.plantgdb.org/GmGDB/). A 1E-20 threshold with the *A. thaliana* query sequence was used to identify the ortholog gene sequences in soybean. Specific primers for each selected gene were designed using the Primer3 software (primer3.ut.ee) and the following thermal profile for qPCR amplifications was used: 95°C for 10 min, 95°C for 15 sec and 60°C for 60 sec, for 40 cycles. Confirmation of the single amplicon in each reaction was performed by a dissociation curve step. Each primer couple was tested at different concentrations from 50 to 500 nM with efficiency close to 100%. Relative expression was estimated through ΔΔCt method between CTRL and treated plants, using *β*-actin of soybean (GLYMA_12G063400) as the housekeeping gene.

Table S1. List of metabolites in soybean plants analyzed by LC-MS/MS.

Compound	KEGG ID	Linearity (R^2)	Transition	Precursor ion	Product ion	Retention time	Polarity	Detected in leaves	Detected in roots
AMINO ACIDS									
Phenylalanine	C00079	0.9998	166.1 -> 120.1	166.1	120.1	2.923	+	Y	Y
Leucine	C00123	0.9986	132.1 -> 86.1	132.1	86.1	3.345	+	Y	Y
Tryptophan	C00078	0.9946	205.1 -> 188.0	205.1	188	3.357	+	Y	Y
Isoleucine	C00407	0.9971	132.1 -> 86.1	132.1	86.1	3.714	+	Y	BDL
Methionine	C00073	0.9993	150.1 -> 104.0	150.1	104	4.198	+	Y	Y
Valine	C00183	0.9997	118.1 -> 72.1	118.1	72.1	4.906	+	Y	Y
Proline	C00148	0.9994	116.1 -> 70.1	116.1	70.1	4.932	+	Y	Y
Tyrosine	C00082	0.9999	182.1 -> 136.1	182.1	136.1	4.968	+	Y	Y
Cysteine	C00097	0.9882	122.0 -> 59.1	122	59.1	5.567	+	Y	Y
Alanine	C00041	0.9997	90.1 -> 44.2	90.1	44.2	6.592	+	Y	Y
Threonine	C00188	0.9996	120.1 -> 74.1	120.1	74.1	6.706	+	Y	Y
Homoserine	C00263	0.9989	120.1 -> 74.1	120.1	74.1	6.891	+	BDL	BDL
Glycine	C00037	0.9998	76.0 -> 30.3	76	30.3	6.972	+	Y	Y
Glutamine	C00064	0.9735	147.1 -> 84.1	147.1	84.1	7.209	+	Y	BDL
Serine	C00065	0.9994	106.1 -> 42.2	106.1	42.2	7.238	+	Y	Y
Asparagine	C00152	0.9997	133.1 -> 87.1	133.1	87.1	7.286	+	Y	Y
Glutamic acid	C00025	0.9970	148.1 -> 84.1	148.1	84.1	7.713	+	Y	Y
Citrulline	C00327	0.9950	176.1 -> 159.1	176.1	159.1	7.855	+	BDL	BDL
Aspartic acid	C00049	0.9991	134.0 -> 74.0	134	74	8.438	+	Y	Y
Histidine	C00135	0.9994	156.1 -> 110.1	156.1	110.1	9.042	+	Y	Y
Arginine	C00062	0.9997	175.1 -> 70.1	175.1	70.1	9.528	+	Y	Y
Lysine	C00047	0.9998	147.1 -> 84.1	147.1	84.1	10.151	+	Y	Y
Ornithine	C00077	0.9999	133.1 -> 70.0	133.1	70	10.272	+	BDL	BDL
Amino acid Internal Standards									
Isoleucine-15N1			133.1 -> 87.1	133.1	87.1	3.713	+		
Methionine-D8			158.1 -> 112.1	158.1	112.1	4.231	+		
Alanine-D3			93.1 -> 47.2	93.1	47.2	6.6	+		
D2 Glycine-110817-2			78.1 -> 32.2	78.1	32.2	6.979	+		
Glutamic acid-15N1			149.1 -> 85.1	149.1	85.1	7.712	+		
D3 Aspartic acid-1			137.1 -> 91.1	137.1	91.1	8.421	+		
D8 Lysine			155.2 -> 92.1	155.2	92.1	10.158	+		

Compound	KEGG ID	Linearity (R^2)	Transition	Precursor ion	Product ion	Retention time	Polarity	Detected in leaves	Detected in roots
ANTIOXIDANTS									
Glutathione reduced	C00051	0.9996	308.1 -> 179.0	308.1	179	1.996	+	BDL	BDL
Gallic acid hydrate	C01424	0.9935	169.0 -> 125.1	169	125.1	4.674	-	BDL	BDL
Chlorogenic acid	C00852	0.9934	353.1 -> 191.1	353.1	191.1	6.168	-	BDL	BDL
Caffeic acid	C01481	0.9921	179.0 -> 135.1	179	135.1	6.54	-	Y	Y
Vanillic acid	C06672	0.9970	167.0 -> 152.1	167	152.1	6.583	-	BDL	BDL
p-Coumaric acid	C00811	0.9639	163.0 -> 119.1	163	119.1	6.958	-	BDL	BDL
2-hydroxycinnamic acid	C01772	0.9958	163.0 -> 119.1	163	119.1	7.125	-	BDL	BDL
Benzoic acid	C00180	0.9987	121.0 -> 77.1	121	77.1	7.43	-	Y	Y
4-(Trifuoromethyl)-cinnamic acid	C00423	0.9981	215.0 -> 171.1	215	171.1	8.23	-	BDL	BDL
L-Dehydroascorbic acid	C00425	0.9976	173.0 -> 158.1	173	158.1	8.324	-	BDL	BDL
Curcumin	C10443	0.9889	367.1 -> 217.1	367.1	217.1	8.327	-	BDL	BDL
α-Tocopherol	C02477	0.9909	431.4 -> 165.1	431.4	165.1	11.274	+	BDL	BDL
ORGANIC ACIDS									
Ascorbic acid	C00072	0.9503	175.0 -> 114.9	175	114.9	2.034	-	Y	BDL
Glycolic acid	C00160	0.9987	75.0 -> 47.0	75	47	2.071	-	BDL	BDL
Malic acid	C00149	0.9979	133.0 -> 114.9	133	114.9	2.156	-	Y	Y
Lactic acid	C00186	0.9991	89.0 -> 43.1	89	43.1	2.272	-	BDL	BDL
Citric acid	C00158	0.9924	191.0 -> 110.8	191	110.8	2.336	-	Y	Y
Succinic acid	C00042	0.9902	117.0 -> 72.9	117	72.9	2.402	-	BDL	BDL
Pyruvic acid	C00022	0.9938	87.0 -> 43.1	87	43.1	2.636	-	BDL	BDL
Glutaric acid	C00489	0.9932	131.0 -> 86.9	131	86.9	2.825	-	BDL	BDL
Fumaric acid	C00122	0.9934	115.0 -> 70.9	115	70.9	2.837	-	Y	Y
Ferulic acid	C01494	0.9911	193.1 -> 178.1	193.1	178.1	5.913	-	BDL	BDL

Y= present, BDL= below detection limit

Table S3. Characterization of 100 μg/ml CdS-QDs suspended in Milli-Q-water or fresh soybean root exudates.

	Milli-Q-Water				**Soybean root exudate**			
	pH	**Hydrodynamic dia. (nm)**	**Zeta-potential (mV)**	**Percent dissolution (24h)**	**pH**	**Hydrodynamic dia. (nm)**	**Zeta-potential (mV)**	**Percent dissolution (24h)**
QD-BARE	6.2 ± 0	550 ± 16	- 18.7 ± 1.2	9.8 ± 0.7	6.5 ± 0	314 ± 5	- 24.4 ± 0.6	5.6 ± 1.6
QD-TOPO	5.6 ± 0	1133 ± 62	- 13.8 ± 0.0	15.3 ± 0.5	6.3 ± 0	1233 ± 13	- 17.5 ± 0.3	1.5 ± 0.1
QD-PVP	7.0 ± 0	950 ± 20	- 4.7 ± 0.3	9.3 ± 0.3	6.9 ± 0	333 ± 4	- 27.6 ± 0.4	4.2 ± 0.3
QD-MAA	6.8 ± 0	306 ± 2	- 22.8 ± 0.6	5.5 ± 0.0	6.7 ± 0	347 ± 2	- 27.7 ± 0.5	4.5 ± 0.3
QD-GLY	7.3 ± 0	884 ± 24	- 12.1 ± 0.1	10.6 ± 0.1	6.6 ± 0	314 ± 3	- 28.0 ± 0.1	2.8 ± 0.5

Table S8. Log-normalized relative fold change in gene expression in the roots and shoots of soybean plants exposed to ION, BULK, and CdS-QDs compared to CTRL.

ROOTS													
	LHY1	BIP3	HIPP22	VIT	PR1	SULTR4;2	PRR5	GGCT2;1	HMA8	NRAMP6	TIP2-1	MT2	MT-1
ION	-0.25	0.54	-2.18	-1.36	5.09	-0.26	-0.02	-0.87	-0.74	0.73	-1.29	-0.41	0.42
BULK	0.91	0.65	-3.11	-0.58	6.02	1.11	-0.49	-1.93	-1.79	-0.18	-1.41	1.28	-1.04
QD-BARE	-0.68	-0.07	-3.24	-1.98	4.03	0.31	-1.10	-2.08	-4.23	-1.56	-2.84	-1.00	-0.22
QD-TOPO	0.81	0.30	-3.61	0.23	5.95	0.68	-0.59	-1.62	-9.65	-3.59	-1.20	0.56	-0.17
QD-PVP	0.47	0.36	-3.51	-1.05	5.86	-0.67	-1.16	-1.90	-3.36	-5.77	-2.56	-0.37	0.49
QD-MAA	0.19	0.19	-1.62	-0.09	6.03	0.93	-0.78	-1.29	-1.07	-6.52	-1.39	0.23	0.96
QD-GLY	0.22	0.79	-2.34	1.04	6.15	-0.39	-2.78	-1.82	-1.81	-6.31	-1.71	0.08	-0.65

SHOOTS														
	LHY1	BIP3	HIPP22	VIT	PR1	SULTR4;2	PRR5	GGCT2;1	ORF31	HMA8	NRAMP6	TIP2-1	MT2	MT-1
ION	1.48	1.46	-1.39	0.18	2.56	2.33	0.94	0.30	1.91	-1.36	0.76	0.85	1.49	3.68
BULK	-1.69	-0.56	-3.28	-1.28	1.34	-1.69	-0.11	-2.08	0.07	-0.99	-0.94	-0.44	0.74	2.37
QD-BARE	-0.43	-1.33	-0.22	0.64	1.59	-0.28	0.57	-1.40	0.48	-0.78	-0.98	-1.06	1.22	3.10
QD-TOPO	-0.79	-0.92	-2.94	0.52	1.59	-1.87	-0.97	-2.16	-0.17	-0.01	-0.82	-1.86	-0.16	2.45
QD-PVP	0.47	-1.06	-2.04	0.90	2.60	4.14	-0.16	-2.91	0.79	0.36	-1.20	-0.78	1.23	2.06
QD-MAA	0.74	0.03	-2.76	0.65	1.56	3.06	0.77	-2.56	0.78	1.49	-1.48	-1.07	1.73	2.36
QD-GLY	-0.72	-0.44	-2.88	1.85	1.06	2.93	-0.23	-1.44	0.92	2.34	-1.76	-0.53	0.54	2.43

Table S9. Cadmium content (μg/g) in the subcellular fractions and whole tissue of root and shoot of soybean plants exposed to 10 μg/mL ION, 100 μg/mL BULK and 200 μg/mL CdS-QDs. Data reused with permission from (3).

	Treatment	Cell wall	Organelle	Membrane	Soluble	Whole tissue (unfractionated)		
ROOT	CTRL	0.2 ± 0.0	21.3 ± 0.0	7.8 ± 0.0	0.0 ± 0.0	0.3±0.11 a		
	ION	61.0 ± 6.4	60.5 ± 6.8	29.2 ± 10.8	2.4 ± 0.6	164.8±47.2 ab		
	BULK	330.4 ± 148.6	228.9 ± 20.5	140.7 ± 26.6	14.0 ± 0.8	639.23±109 bc		
	QD-BARE	801.2 ± 26.4	737.4 ± 10.4	788.6 ± 327.5	49.1 ± 10.0	1199.6±216.4 cd		
	QD-TOPO	469.4 ± 94.2	376.6 ± 82.4	685.1 ± 280.2	34.2 ± 0.5	1066.9±163.8 cd		
	QD-PVP	552.8 ± 141.3	878.3 ± 118.1	348.1 ± 47.0	32.7 ± 4.1	1223.0±38.5 d		
	QD-MAA	1202.3 ± 128.4	619.5 ± 137.2	322.0 ± 56.2	45.2 ± 7.6	1287.1±164.4 d		
	QD-GLY	620.4 ± 42.8	535.2 ± 96.6	344.5 ± 86.0	33.8 ± 3.5	989.6±79.1 cd		
						Total shoot	**Stem**	**Leaf**
SHOOT	CTRL	0.0 ± 0.0	0.1 ± 0.0	0.2 ± 0.0	0.0 ± 0.0	0.1±0.0 a	0.1±0.0 a	0.1±0.0 a
	ION	4.7 ± 0.6	3.9 ± 0.1	3.6 ± 1.7	2.0 ± 0.2	17.5±2.0 ab	26.6±3.9 a	5.1±2.0 a
	BULK	8.1 ± 3.1	8.1 ± 1.9	9.5 ± 6.2	2.3 ± 0.4	34.2±9.2 ab	47.7±13.5 ab	6.1±2.4 a
	QD-BARE	5.8 ± 1.4	5.5 ± 1.7	5.0 ± 2.6	2.6 ± 1.1	24.7±2.6 ab	39.2±4.2 a	0.8±0.2 a
	QD-TOPO	14.6 ± 2.3	11.8 ± 3.1	16.1 ± 4.8	4.3 ± 0.3	29.1±9.1 ab	44.1±12.1 ab	1.5±0.2 a
	QD-PVP	28.5 ± 10.1	27.7 ± 9.6	34.9 ± 22.5	6.2 ± 2.0	73.7±13.4 c	99.1±16.3 c	4.8±1.2 a
	QD-MAA	9.7 ± 2.0	10.3 ± 1.5	7.6 ± 0.3	3.3 ± 0.6	24.5±3.4 ab	37.9±5.1 a	2.1±1.0 a
	QD-GLY	11.5 ± 4.3	12.0 ± 6.5	9.5 ± 6.3	4.2 ± 1.4	60.2±9.0 bc	92.5±16.4 bc	3.9±0.8 a

Table S10. Fold change in the abundance of differentially accumulated metabolites in roots from soybean plants exposed to ION, BULK, and CdS-QDs compared to CTRL, estimated by ANOVA and Fisher's LSD post hoc analysis ($p \leq 0.05$). Red cells represent significant upregulation and green cells represent significant downregulation. Numbers in **bold** represent fold change ≥ 2.0.

Compound name	***p*-value**	**FDR**	**Fold change (Treatment vs CTRL)**						
			ION	**BULK**	**QD-BARE**	**QD-TOPO**	**QD-PVP**	**QD-MAA**	**QD-GLY**
Alanine	7.54E-03	1.16E-02	**-3.12**	**-2.66**	-1.00	-1.42	-1.95	-1.11	-1.29
Arginine	3.03E-04	2.32E-03	**-3.93**	-1.17	1.74	1.22	1.74	1.86	1.18
Asparagine	3.70E-02	4.05E-02	**-2.51**	-1.40	-1.33	**-2.32**	**-2.00**	-1.76	**-2.11**
Aspartic acid	7.08E-03	1.16E-02	-1.94	-1.10	1.66	1.07	-1.25	1.51	1.23
Benzoic acid	3.68E-03	9.20E-03	-1.91	-1.48	**-2.50**	**-2.02**	**-2.07**	**-2.41**	**-3.69**
Caffeic acid	3.10E-02	3.76E-02	-1.44	-1.38	-1.46	-1.76	-1.86	-1.54	-1.87
Citric acid	7.16E-04	4.11E-03	-1.60	-1.29	1.08	-1.27	-1.60	1.70	1.25
Cysteine	1.90E-02	2.73E-02	-1.45	-1.46	-1.76	-1.81	-1.84	-1.46	**-2.05**
Fumaric acid	2.71E-02	3.46E-02	1.09	1.13	-1.12	1.06	-1.50	1.16	1.68
Glutamic acid	9.97E-07	2.29E-05	**2.55**	**4.30**	**9.39**	**11.11**	**4.85**	**21.19**	**11.90**
Glycine	4.00E-03	9.20E-03	**-2.51**	-1.90	-1.46	-1.77	**-2.19**	1.14	**-2.06**
Histidine	2.19E-02	2.96E-02	**-2.48**	-1.26	1.14	-1.33	-1.53	-1.07	-1.41
Leucine	3.69E-02	4.05E-02	**-2.32**	**-2.10**	-1.69	-1.77	**-2.42**	-1.76	**-2.23**
Lysine	9.02E-04	4.15E-03	**-2.79**	-1.40	1.46	1.29	-1.14	1.45	-1.21
Methionine	5.85E-03	1.04E-02	-1.78	-1.69	-1.89	-1.96	**-2.12**	-1.52	**-2.22**
Phenylalanine	5.85E-03	1.04E-02	**-4.29**	**-2.32**	-1.22	-1.41	**-2.66**	1.16	-1.59
Proline	3.85E-03	9.20E-03	**-3.61**	**-3.41**	1.23	-1.06	**-2.23**	1.26	1.14
Serine	4.61E-02	4.82E-02	**-2.69**	**-2.30**	-1.11	-1.38	**-2.77**	-1.22	-1.60
Threonine	2.29E-03	7.53E-03	**-3.42**	**-2.63**	-1.59	**-2.18**	**-3.04**	-1.56	**-2.18**
Tryptophan	1.30E-04	1.50E-03	-1.90	1.68	2.69	**2.78**	1.94	**2.19**	**2.83**
Tyrosine	1.19E-03	4.54E-03	-1.85	1.17	1.43	1.83	-1.51	**3.05**	1.68
Valine	4.97E-03	1.04E-02	**-5.97**	**-5.11**	**-2.41**	**-2.85**	**-5.10**	**-2.46**	**-3.67**

Table S11. Fold change in the abundance of differentially accumulated metabolites in leaves from soybean plants exposed to ION, BULK, and CdS-QDs compared to CTRL, estimated by ANOVA and Fisher's LSD post hoc analysis ($p \leq 0.05$). Red cells represent significant upregulation and green cells represent significant downregulation. Numbers in **bold** represent fold change ≥ 2.0.

Compound name	***p*-value**	**FDR**	**Fold change (Treatment vs CTRL)**						
			ION	**BULK**	**QD-BARE**	**QD-TOPO**	**QD-PVP**	**QD-MAA**	**QD-GLY**
Alanine	1.08E-02	2.00E-02	-1.27	-1.05	1.38	1.75	1.61	1.87	1.63
Arginine	1.34E-02	2.32E-02	-1.35	1.08	1.20	1.61	1.97	-1.37	-1.52
Asparagine	2.89E-02	4.17E-02	1.03	1.09	1.06	1.19	1.25	1.22	1.12
Aspartic acid	8.01E-03	1.60E-02	1.08	-1.02	1.07	1.47	1.28	1.55	1.47
Glutamic acid	1.23E-07	3.19E-06	-1.07	1.01	1.58	1.64	**-2.24**	1.10	-1.01
Glutamine	2.43E-02	3.72E-02	-1.80	-1.95	1.14	-1.41	1.76	1.41	1.13
Glycine	1.55E-05	2.01E-04	-1.17	1.23	1.51	1.98	**2.09**	1.55	1.42
Histidine	1.06E-03	3.07E-03	1.05	1.12	1.33	1.47	1.65	1.23	1.19
Isoleucine	2.16E-02	3.51E-02	-1.78	-1.27	1.90	1.96	1.54	1.66	1.12
Leucine	1.39E-03	3.63E-03	-1.55	-1.14	1.93	1.86	1.86	1.24	-1.12
Lysine	6.76E-04	2.30E-03	-1.19	1.27	**2.24**	**2.65**	**3.43**	1.14	-1.32
Malic acid	2.98E-04	1.29E-03	1.10	1.12	-1.07	1.28	-1.11	1.63	1.65
Methionine	3.44E-03	8.12E-03	-1.37	-1.37	1.51	1.40	1.50	1.22	1.01
Proline	2.56E-04	1.29E-03	-1.94	-1.50	**3.77**	**2.51**	1.75	**3.43**	**2.36**
Serine	5.36E-03	1.16E-02	-1.22	-1.04	**2.10**	**2.60**	**2.16**	**2.44**	**2.12**
Threonine	5.33E-05	4.62E-04	-1.18	1.15	**2.36**	**2.72**	**2.32**	**2.20**	1.82
Tyrosine	1.37E-04	8.92E-04	-1.63	-1.38	**2.54**	**2.79**	1.62	1.79	1.25
Valine	7.06E-04	2.30E-03	-1.82	-1.12	**4.22**	**4.10**	**3.63**	**2.82**	1.79

Table S13. Element contents (μg/g) in the tissues of soybean plants exposed to 10 μg/mL ION, 100 μg/mL BULK and 200 μg/mL CdS-QDs. Data reused and printed with the permission from Majumdar et al. (3)

TREATMENTS	**ROOT**				**STEM**	**LEAF**
	Magnesium	**Sodium**	**Iron**	**Manganese**	**Copper**	**Copper**
CTRL	6616.2±1664.5 ab	1861.2±279.8 ab	5236.5±1285.7 ab	85.8±8.7 ab	11.8±0.9 ab	32.6±4.0 ab
ION	14373.0±5821.9 a	2244.6±928.1 a	10569.9±3949.2 a	165.6±61.4 a	13.7±1.7 ab	33.3±3.3 a
BULK	6129.4±806.9 ab	1224.9±288.1 ab	4873.4±698.6 ab	91.4±15.7 ab	12.1±1.0 ab	18.0±1.8 abc
QD-BARE	3962.5±809.4 b	1042.1±440.1 ab	3016.4±580.1 b	59.9±9.8 ab	10.0±2.0 ab	12.8±0.7 c
QD-TOPO	3470.1±989.4 b	1161.1±473.4 ab	3048.3±698.7 b	63.4±16.4 ab	19.0±7.1 a	16.1±1.4 c
QD-PVP	2651.5±123.9 b	259.2±46.4 b	2113.9±109.7 b	57.3±1.3 ab	13.1±1.5 ab	21.4±3.0 abc
QD-MAA	3463.7±1346.9 b	1237.1±274.3 ab	2122.3±697.2 b	62.4±9.3 ab	7.9±0.5 b	14.0±1.0 c
QD-GLY	2450.4±192.8 b	813.6±121.5 ab	2062.4±160.7 b	43.1±3.4 b	12.2±2.0 ab	15.2±1.4 c

Figure S1. Principal component analysis of the identified proteins in the soybean roots exposed to CTRL, 10 µg/mL ION, 100 µg/mL BULK and 200 µg/mL CdS-QDs (QD-BARE, QD-TOPO, QD-PVP, QD-MAA, QD-GLY).

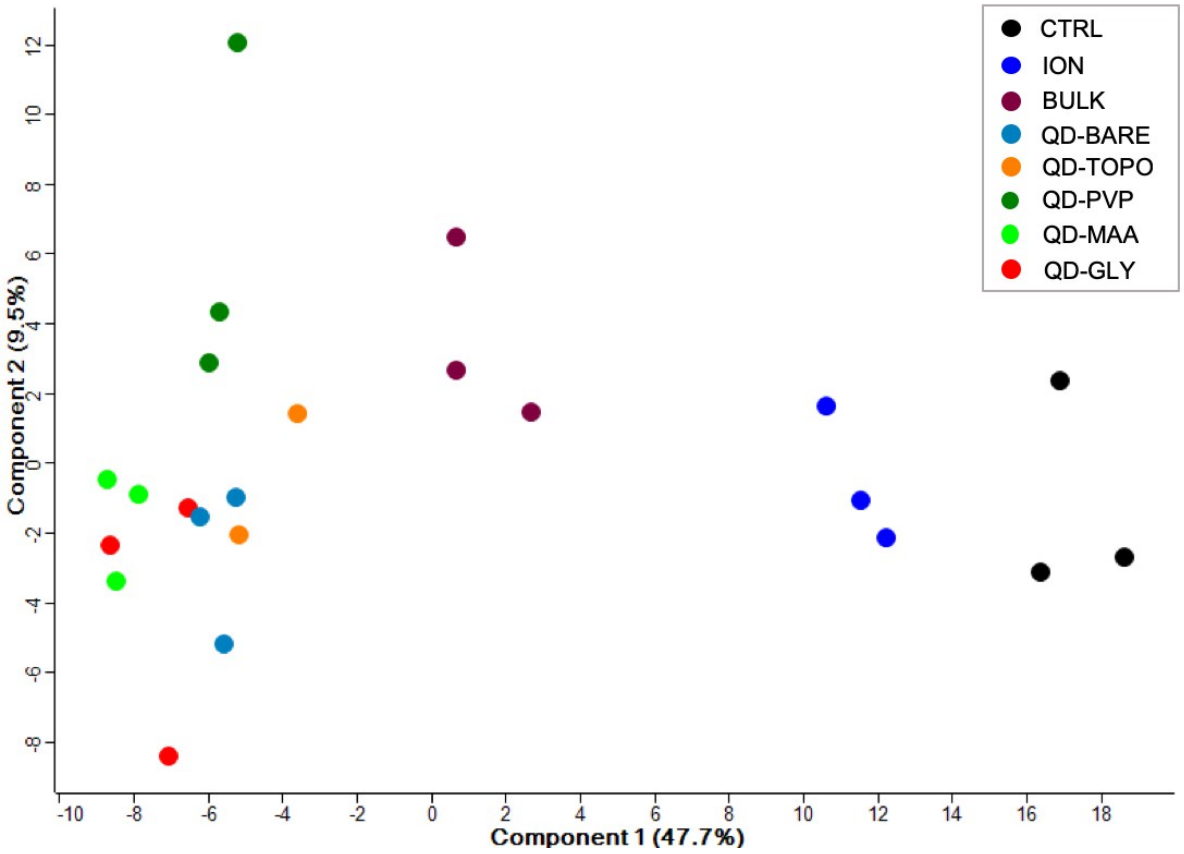
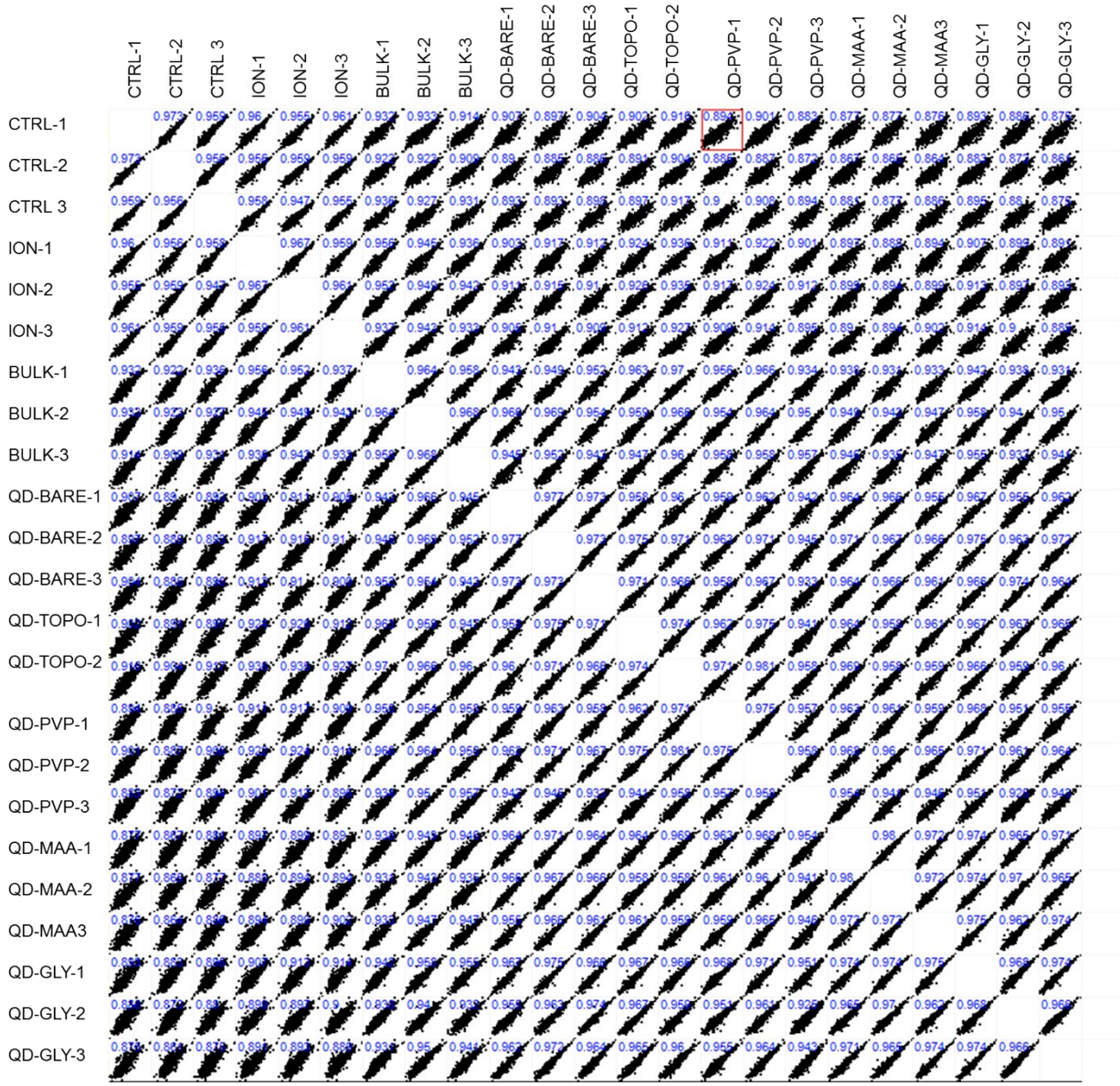


Figure S2. Multi-scatter plots of the identified proteins (including Pearson's coefficient) in the soybean roots exposed to CTRL, 10 μg/mL ION, 100 μg/mL BULK and 200 μg/mL CdS-QDs (QD-BARE, QD-TOPO, QD-PVP, QD-MAA, QD-GLY).



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