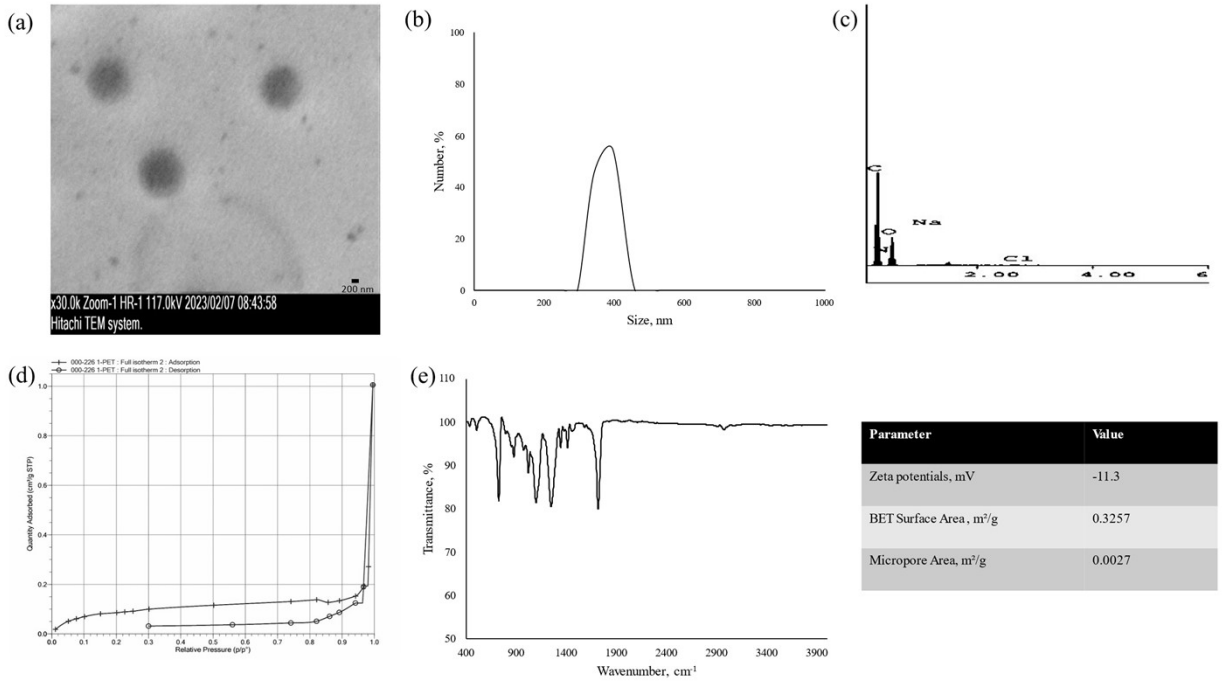
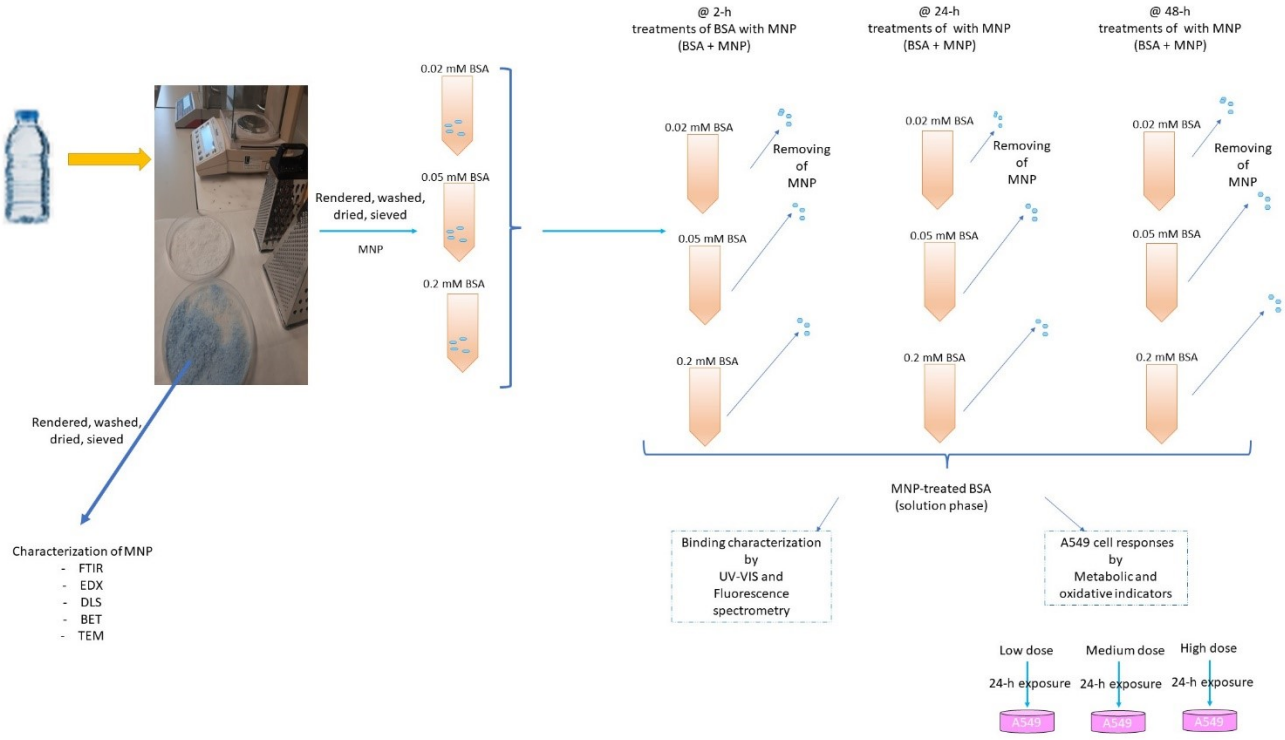
Supplementary Materials

Supplementary Figure 1. Physichemical characteristics of PET MNPs (a) TEM, (b) particle size distribution, (c) EDX spectrum, (d) BET sorption/desorption isotherms, (e) FTIR spectrum (Figures from our previous work (https://doi.org/10.1002/tox.24366) [34]).

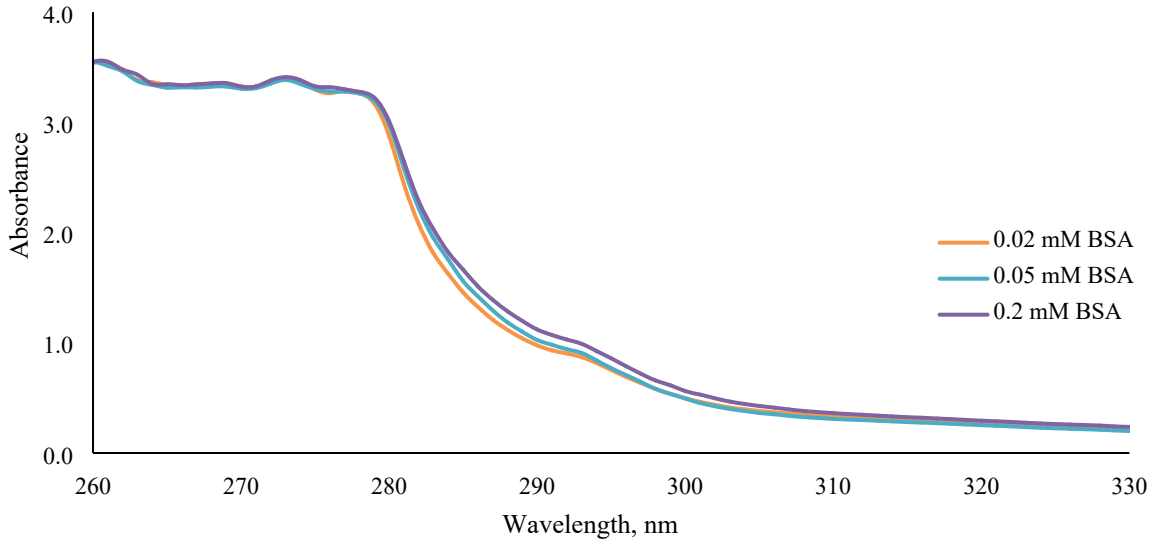


Parameter	Value
Zeta potentials, mV	-11.3
BET Surface Area , m^2/g	0.3257
Micropore Area, m^2/g	0.0027

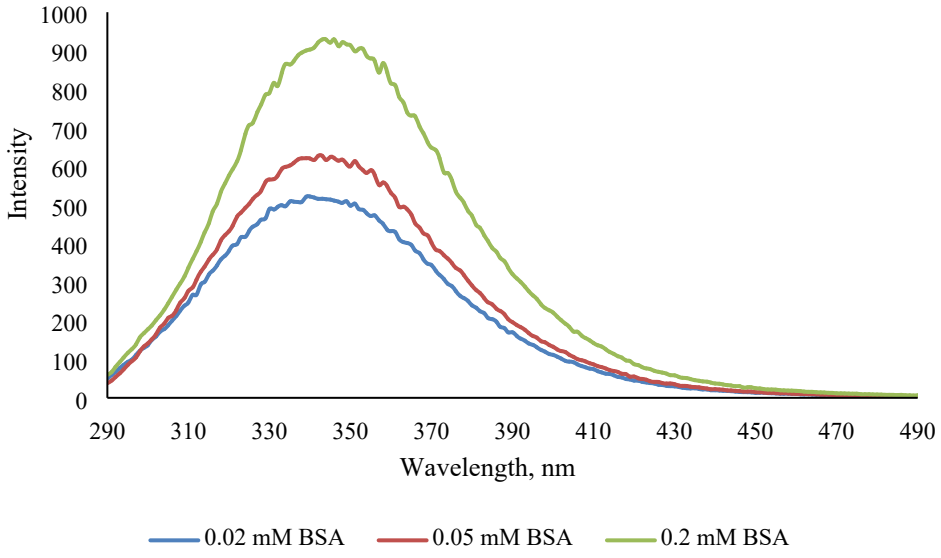
Supplementary Figure 2. Experimental set-up for the MNP-BSA interaction



Supplementary Figure 3. UV-VIS spectra of BSA standards at the concentration of 0.02 mM, 0.05 mM and 0.2 mM.



Supplementary Figure 4. Fluorescence spectra of BSA standards at the concentration of 0.02 mM, 0.05 mM and 0.2 mM.



Supplementary Figure 5. Correlation and heat map between the cytotoxic (MTT, CCK-8 and LDH levels) and oxidative stress indicators of A549 cell. (a) PET MNP treatment stage relationship, (b) BSA concentration relationship

(a)

Parameters	2 h PET MNP treatment			24 h PET MNP treatment			48 h PET MNP treatment		
	Low	Medium	High	Low	Medium	High	Low	Medium	High
MTT-CCK	0.87	-0.03	0.99	-0.99	0.02	-0.46	1.00	0.98	0.95
MTT-LDH	0.97	0.92	0.83	-0.58	0.84	0.65	-0.37	1.00	-0.18
MTT-ROS	0.36	0.93	0.51	-0.37	-0.83	-0.47	0.68	-0.70	-0.70
MTT-AOX	-0.34	-0.70	0.22	-0.91	0.30	-0.06	0.94	-0.51	0.37
MTT-SOD	0.97	-0.92	0.69	-0.24	-0.92	0.90	0.80	-0.84	-0.92
MTT-GLU	-0.93	0.24	0.82	0.90	0.65	0.80	-0.22	-0.72	0.66
CCK-ROS	0.74	0.98	0.56	-0.01	-0.73	-0.42	0.68	-0.74	-0.83
CCK-AOX	-0.75	-0.70	0.34	0.96	0.96	0.91	0.94	-0.65	0.64
CCK-SOD	0.97	0.42	0.60	0.12	0.37	-0.02	0.80	-0.93	-0.76
CCK-GLU	-0.99	0.96	0.74	-0.95	0.77	0.17	-0.49	-0.63	0.93
LDH-CCK	0.97	0.36	0.75	0.48	0.56	-0.98	-0.38	0.99	0.14
LDH-ROS	0.51	0.90	-0.27	-0.53	-0.41	-0.74	0.44	-0.75	0.25
LDH-AOX	-0.56	-0.92	-0.36	0.20	0.77	-0.80	-0.05	-0.57	0.85
LDH-SOD	1.00	-0.69	0.98	0.93	-0.57	0.24	0.25	-0.88	0.54
LDH-GLU	-0.99	0.60	1.00	-0.17	0.96	0.05	-0.62	-0.70	-0.24

(b)

	0.02 mM BSA			0.05 mM BSA			0.2 mM BSA		
	Low	Medium	High	Low	Medium	High	Low	Medium	High
MTT-CCK	0.99	0.99	0.97	0.64	0.97	0.63	0.97	0.99	0.90
MTT-LDH	-0.58	0.31	0.98	0.88	0.27	0.65	0.33	0.66	0.90
MTT-ROS	0.55	-0.33	-0.63	-0.73	-0.72	-0.51	-0.29	-0.38	0.32
MTT-AOX	0.86	0.56	0.64	-0.40	0.60	0.66	0.85	-0.47	0.14
MTT-SOD	-0.63	0.72	-0.25	0.24	0.92	0.90	0.81	0.86	-0.73
MTT-GLU	0.00	-0.89	0.18	0.52	0.36	0.44	0.99	0.75	0.62
CCK-ROS	0.46	-0.23	-0.43	-0.83	-0.54	-0.82	-0.44	-0.30	0.43
CCK-AOX	0.90	0.49	0.44	0.36	0.65	0.48	0.79	-0.35	0.49
CCK-SOD	-0.69	0.72	-0.09	0.50	0.79	0.25	0.66	0.91	-0.57
CCK-GLU	-0.04	-0.89	0.26	0.91	0.43	0.92	0.99	0.79	0.22
LDH-CCK	-0.49	0.27	0.95	0.29	0.36	-0.18	0.19	0.71	0.62
LDH-ROS	-0.94	-0.26	-0.65	-0.62	-0.24	0.23	-0.31	-0.50	0.13
LDH-AOX	-0.15	0.86	0.63	-0.77	-0.39	0.25	-0.05	0.01	-0.26
LDH-SOD	-0.17	-0.38	-0.10	-0.20	0.17	0.87	0.77	0.56	-0.76
LDH-GLU	-0.24	-0.65	0.36	0.31	0.99	-0.38	0.31	0.99	0.90

Supplementary Figure 6. Correlation analysis between A549 cell responses and binding and oxidative characteristics of BSA. (a) PET MNP treatment stage relationship, (b) BSA concentration relationship

(a)

Cytotoxicity and oxidative parameters	Exposure concentration to A549	Ksv			Folding			Aromatic side chain			Zeta potentials			DTT			ROS		
		2 h	24 h	48 h	2 h	24 h	48 h	2 h	24 h	48 h	2 h	24 h	48 h	2 h	24 h	48 h	2 h	24 h	48 h
MTT	low	1.00	-0.70	0.96	0.65	-0.82	0.92	0.90	-0.99	0.98	0.91	0.76	0.99	0.98	-0.83	-0.39	0.94	-0.76	0.85
	medium	0.47	-0.89	0.88	-0.43	-0.58	0.93	0.77	-0.98	0.83	0.00	0.93	0.83	0.57	-0.97	0.36	0.06	-0.93	0.98
	high	-0.89	-0.32	0.75	-0.89	-0.99	0.66	-0.66	-0.83	0.81	-1.00	0.41	0.81	-0.83	-0.50	-0.75	-1.00	-0.40	0.54
CCK	low	0.91	0.60	0.96	0.20	0.88	0.92	1.00	0.97	0.98	0.60	-0.68	0.98	0.95	0.75	-0.40	0.65	0.67	0.85
	medium	-0.89	0.44	0.95	-0.89	-0.82	0.98	-0.67	-0.21	0.92	-1.00	-0.34	0.91	-0.84	0.24	0.18	-1.00	0.35	1.00
	high	-0.94	0.99	0.92	-0.83	0.31	0.86	-0.75	0.87	0.95	-0.99	-1.00	0.96	-0.90	1.00	-0.51	-1.00	1.00	0.77
LDH	low	0.99	0.99	-0.11	0.45	0.01	0.01	0.98	0.69	-0.20	0.78	-0.97	-0.21	1.00	0.94	1.00	0.82	0.97	0.17
	medium	0.09	-0.51	0.91	-0.75	-0.93	0.96	0.45	-0.93	0.87	-0.40	0.59	0.87	0.21	-0.67	0.28	-0.34	-0.58	0.99
	high	-0.49	-0.93	0.52	-0.99	-0.51	0.62	-0.13	-0.96	0.44	-0.85	0.96	0.43	-0.38	-0.99	0.78	-0.81	-0.96	0.74
ROS	low	0.50	-0.31	0.83	-0.40	0.89	0.89	0.79	0.34	0.78	0.03	0.22	0.77	0.60	-0.11	0.44	0.09	-0.23	0.95
	medium	-0.50	-0.39	-0.96	-0.99	0.85	-0.91	-0.15	0.26	-0.98	-0.85	0.30	-0.98	-0.40	-0.20	0.41	-0.82	-0.31	-0.84
	high	-0.58	-0.67	-0.92	-1.00	0.62	-0.86	-0.24	-0.08	-0.95	-0.90	0.60	-0.95	-0.48	-0.51	0.52	-0.87	-0.60	-0.77
Antiox	low	-0.41	0.34	1.00	0.49	0.98	1.00	-0.72	0.85	0.99	0.08	-0.43	0.99	-0.51	0.53	-0.07	0.01	0.43	0.98
	medium	0.30	0.17	-0.86	0.95	-0.95	-0.79	-0.07	-0.48	-0.90	0.72	-0.07	-0.90	0.19	-0.04	0.62	0.68	0.08	-0.68
	high	-0.64	0.97	0.89	0.24	-0.10	0.94	-0.88	0.60	0.85	-0.19	-0.94	0.84	-0.72	0.89	0.33	-0.25	0.94	0.98
GR	low	-0.96	-0.31	-0.71	-0.33	-0.99	-0.79	-1.00	-0.83	-0.64	-0.70	0.40	-0.63	-0.98	-0.50	-0.61	-0.75	-0.39	-0.88
	medium	-0.74	-0.24	-0.35	-0.98	-1.00	-0.47	-0.44	-0.79	-0.27	-0.97	0.33	-0.26	-0.66	-0.43	-0.88	-0.95	-0.32	-0.60
	high	-0.47	0.32	0.71	-0.99	-0.89	0.61	-0.11	-0.33	0.77	-0.83	-0.22	0.77	-0.36	0.12	-0.80	-0.80	0.23	0.48
SOD	low	0.99	0.86	0.93	0.45	-0.36	0.97	0.98	0.37	0.90	0.78	-0.81	0.89	1.00	0.74	0.23	0.82	0.81	1.00
	medium	-0.78	1.00	-1.00	0.04	0.23	-0.98	-0.96	0.83	-1.00	-0.39	-1.00	-1.00	-0.85	0.99	0.20	-0.45	1.00	-0.94
	high	-0.29	0.14	-0.44	-0.94	-0.96	-0.33	0.08	-0.50	-0.52	-0.71	-0.04	-0.53	-0.18	-0.07	0.93	-0.67	0.05	-0.17

(b)

Cytotoxicity and oxidative parameters	Exposure concentration to A549	Ksv			Folding			Aromatic side chain			Zeta potentials			ROS			DTT		
		0.02 mM	0.05 mM	0.2 mM	0.02 mM	0.05 mM	0.2 mM	0.02 mM	0.05 mM	0.2 mM	0.02 mM	0.05 mM	0.2 mM	0.02 mM	0.05 mM	0.2 mM	0.02 mM	0.05 mM	0.2 mM
MTT	low	0.88	0.76	-0.63	0.90	-0.35	-0.50	0.23	-0.03	-0.38	0.25	-0.50	0.20	0.92	-0.65	0.57	0.44	-0.82	-0.77
	medium	-0.64	-0.63	0.71	-0.60	-0.64	0.81	0.91	-0.37	0.88	0.90	-0.77	1.00	-0.57	-0.36	0.88	-0.97	-0.58	-0.72
	high	0.46	0.02	-0.59	0.50	0.47	-0.47	0.74	0.73	-0.34	0.75	0.32	0.24	0.53	-1.00	0.61	-0.15	-0.97	-0.80
CCK	low	0.30	0.99	-0.95	0.25	-0.82	-0.89	-1.00	-0.59	-0.82	-1.00	-0.90	-0.35	0.22	-0.11	0.04	0.80	-0.36	-0.31
	medium	0.89	-0.10	-0.50	0.91	-1.00	-0.37	0.20	-0.96	-0.24	0.22	-0.97	0.34	0.93	0.53	0.69	0.46	0.30	-0.85
	high	-0.67	-0.40	-0.70	-0.71	0.80	-0.59	-0.54	0.95	-0.47	-0.56	0.68	0.10	-0.73	-0.91	0.49	-0.11	-0.78	-0.70
LDH	low	0.99	1.00	0.76	1.00	-0.82	0.85	-0.12	-0.68	0.91	-0.10	-0.91	0.98	1.00	-0.10	0.84	0.72	-0.35	-0.66
	medium	-0.24	0.90	0.81	-0.19	-0.58	0.89	1.00	-0.61	0.95	1.00	-0.71	0.97	-0.16	-0.44	0.79	-0.76	-0.65	-0.60
	high	0.58	-0.08	0.01	0.62	-0.42	-0.14	0.63	1.00	-0.27	0.65	-0.26	-0.76	0.65	1.00	-0.96	0.00	0.98	1.00
ROS	low	-1.00	-1.00	-0.90	0.59	0.86	-0.83	0.29	0.66	-0.74	0.51	-0.10	-0.62	-0.99	0.02	0.16	-0.83	0.27	-0.41
	medium	-0.92	-0.99	-0.04	0.07	0.78	-0.18	-0.15	0.55	-0.32	-0.27	-0.67	-0.34	-0.94	0.16	-0.97	-0.51	0.41	1.00
	high	-0.93	-1.00	-0.95	-0.37	0.83	-0.98	-0.10	0.61	-1.00	-0.38	-0.31	0.06	-0.96	0.09	-0.58	-0.55	0.34	0.34
Antiox	low	0.92	-0.83	-0.93	0.88	0.45	-0.87	-0.62	0.14	-0.79	0.36	0.81	0.63	0.89	0.57	0.08	0.97	0.76	-0.34
	medium	0.33	0.08	0.70	0.74	-0.56	0.59	0.83	-0.79	0.47	0.88	-0.16	-0.28	0.40	1.00	-0.49	-0.29	0.94	0.70
	high	0.99	0.95	-0.98	0.36	-0.98	-0.95	-0.10	-0.87	-0.90	0.25	-0.22	-0.33	1.00	0.31	-0.11	0.70	0.06	-0.16
GR	low	-0.61	0.49	0.35	-0.16	0.00	0.21	0.93	0.32	0.07	0.70	-0.21	-0.40	-0.54	0.08	0.71	-0.96	-0.17	-0.87
	medium	0.53	-0.56	-0.70	-0.89	0.89	-0.80	-0.96	0.99	-0.87	-0.90	0.20	-0.88	0.46	-0.44	0.69	0.92	-0.65	-0.47
	high	-0.46	0.61	-0.71	0.11	-0.14	-0.80	0.98	0.18	-0.88	0.90	-0.47	-0.91	-0.39	-0.33	-0.39	-0.89	-0.56	0.62
SOD	low	-0.62	0.96	-0.86	-0.98	-0.69	-0.92	-0.60	-0.43	-0.97	-0.79	-0.64	0.10	-0.68	0.98	0.97	-0.04	1.00	-1.00
	medium	0.70	0.64	-0.20	0.74	-0.17	-0.34	-0.87	0.15	-0.47	-0.01	-0.56	0.25	0.65	0.57	-0.96	0.99	0.34	1.00
	high	-0.79	0.22	-0.03	-0.14	0.29	0.12	0.80	0.58	0.26	0.56	-0.14	0.99	-0.74	0.91	-0.97	-1.00	0.78	0.88