

## **Supporting Information**

### **Cytotoxicity induction by the oxidative reactivity of nanoparticles revealed by a combinatorial GNP library with diverse redox properties**

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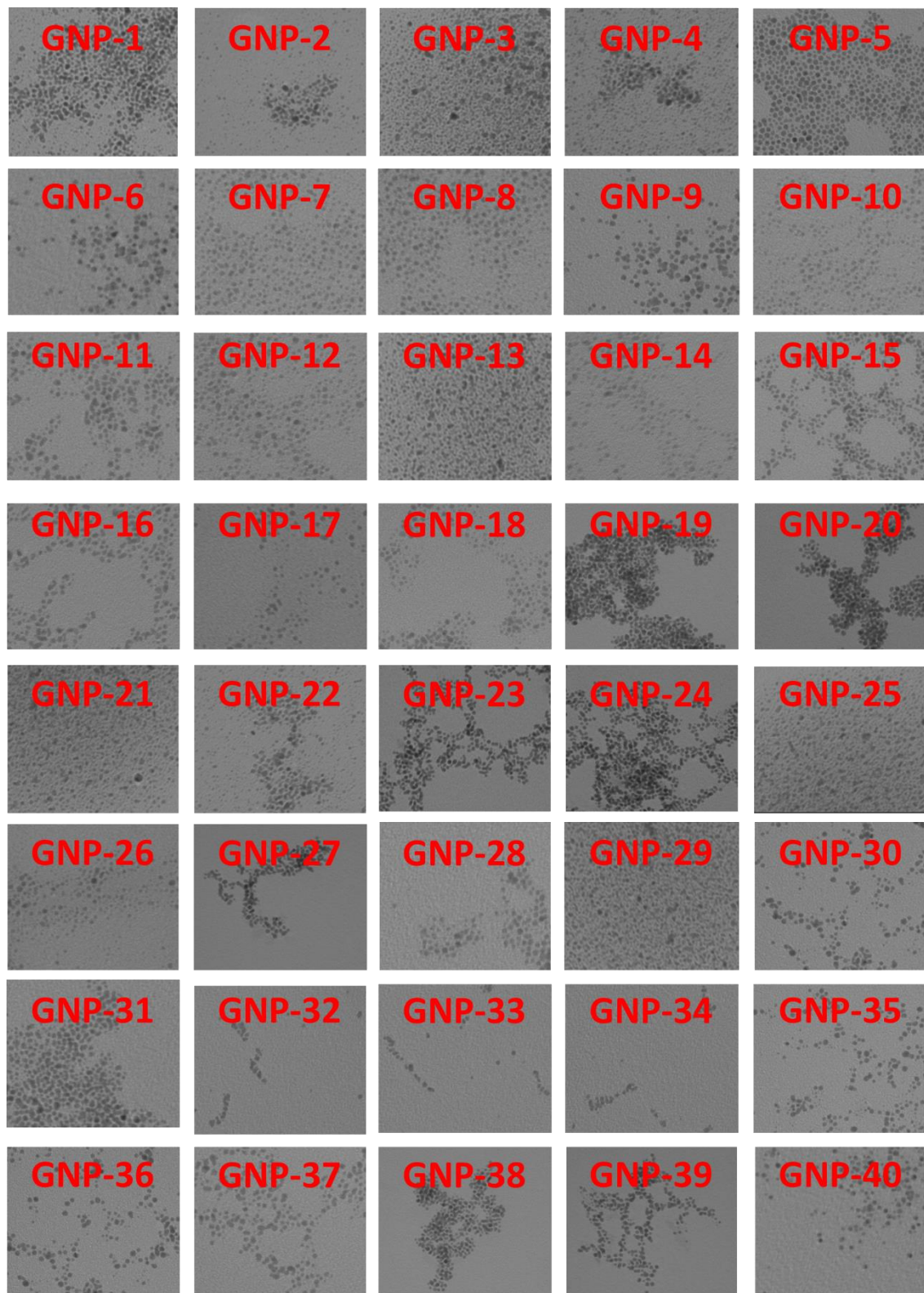
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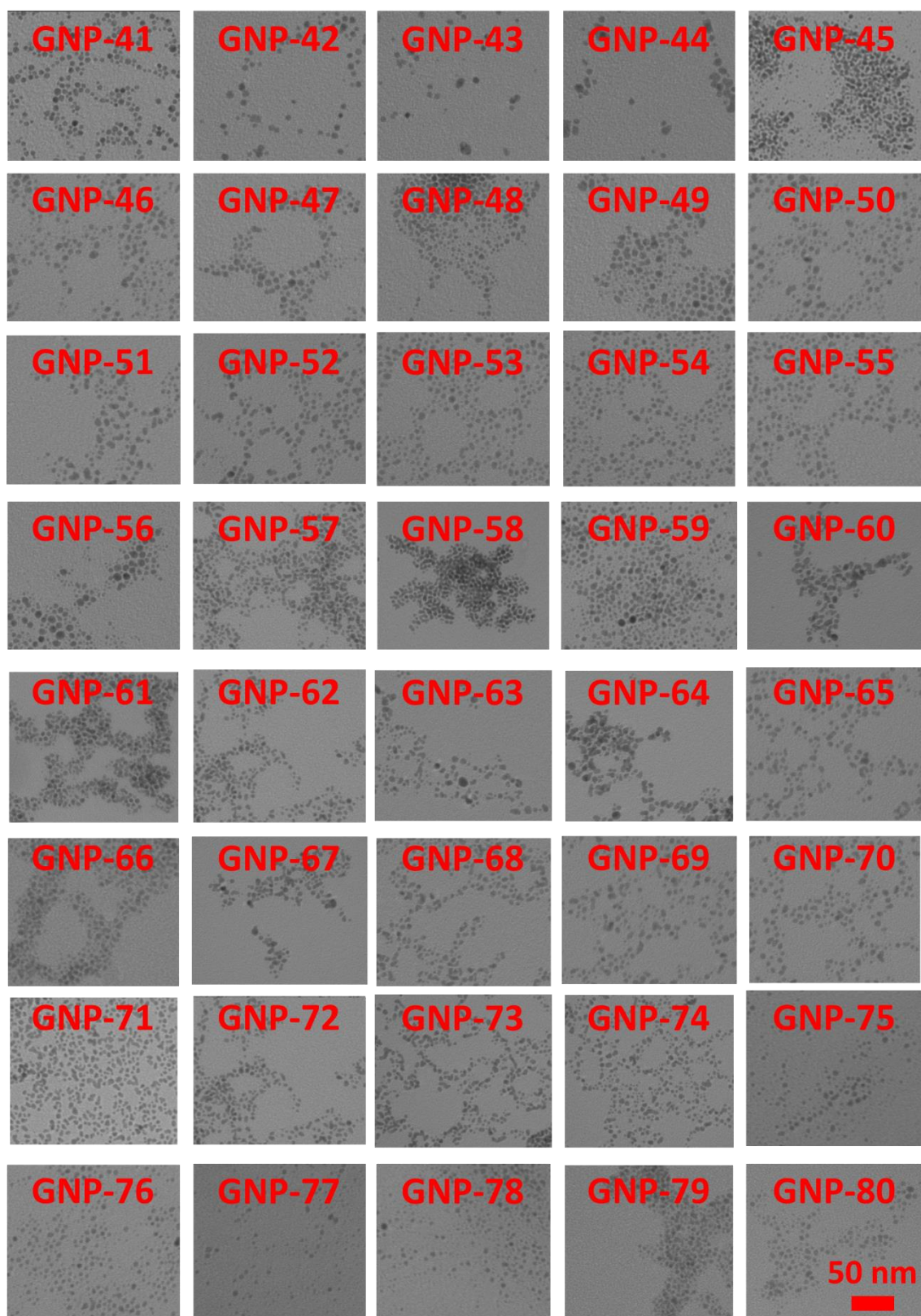
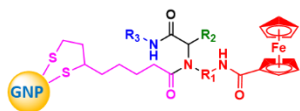


Figure S1. TEM images of 80 GNPs in the whole library.

a



Log P

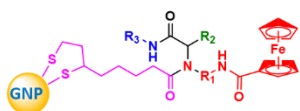
		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		0.99	0.52	-0.5	0.87	0.69
		1.35	0.57	-0.9	0.68	0.77
		0.91	0.3	-0.7	0.59	-0.43
		0.63	-1.3	2.39	1.79	0.42

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		0.07	-0.11	0.02	-0.41	0.47
		0.84	0.45	0.75	0.89	0.27
		0.33	0.91	0.85	0.24	0.37
		0.91	0.51	0.98	0.77	0.32

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		-0.61	0.88	0.74	-0.51	0.78
		-0.44	0.55	0.21	0.18	0.76
		0.58	-0.08	0.33	-0.16	0.77
		0.68	0.76	0.74	0.74	0.76

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		1.66	0.55	0.76	1.09	0.26
		0.82	0.68	1.27	0.23	-0.11
		0.83	0.52	-0.1	0.62	-0.5
		0.36	0.92	0	0.92	-0.3

b



Zeta potential (mV)

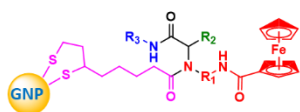
		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		-8.3	-25.6	-38.5	-39.4	-29.7
		0	-27.3	-30.9	-28.1	-44.7
		-7.3	-31.5	-20.1	-58.6	-32
		-5.6	3.5	-3.9	-50.9	-27

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		-31.4	-40.7	-43.3	-40.6	-33
		-36.3	-43.1	-39.7	-36.7	-32.3
		25.4	-24.1	-33.2	-28.7	-26.7
		-30	-10.9	-8.7	-14.9	-19.1

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		-37	-45.5	-34.3	-51	-14.9
		-36.3	-19	-27.4	-51.5	-22.7
		-41.2	-35	-31.4	-40.1	-7.6
		-1.2	15.5	4.8	-28	-19.4

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		15.4	-13.8	-18.9	1	-29.9
		6.3	-23.7	-21.5	1.8	-13.3
		-6.4	-24.9	-18.3	-26.3	-32.3
		-20.4	-37	-30.4	-34.7	-26.3

c



Number of ligands per particle (GNPs)

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		314	337	318	342	309
		295	254	308	332	300
		303	346	263	265	313
		272	297	321	299	330

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		278	334	324	284	284
		317	314	300	276	270
		283	341	312	286	296
		279	259	255	281	333

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		315	341	323	323	335
		274	300	282	359	308
		294	329	352	341	272
		284	342	295	350	240

		R <sub>2</sub>				
		R <sub>3</sub> =				
R <sub>1</sub>						
		308	328	285	329	307
		324	300	271	277	304
		313	314	293	314	350
		313	257	265	301	277



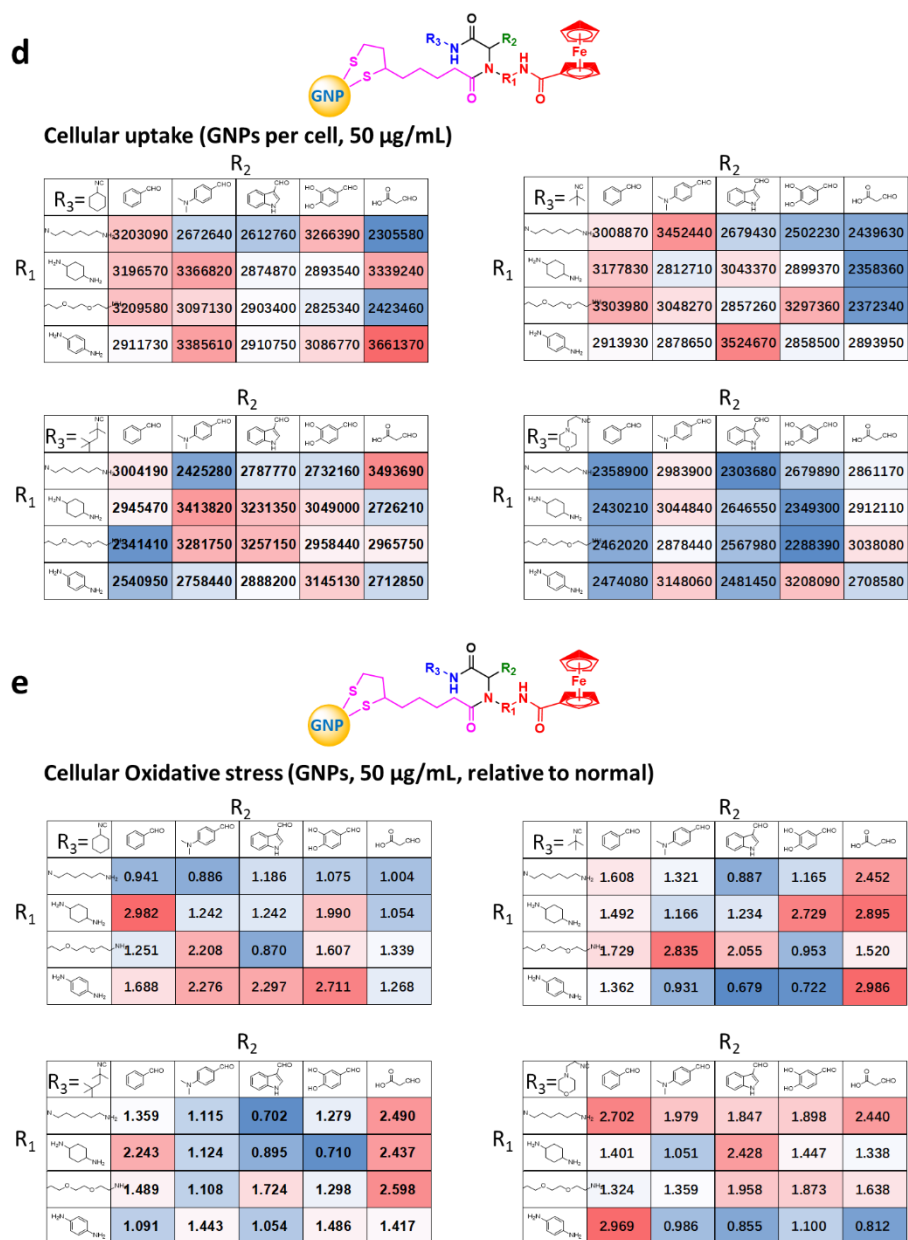


Figure S2. The characterization of physicochemical properties and biological effects of 80 GNPs in the whole library. (a) Log P value, (b) Zeta potential, (c) Number of ligands per GNP, (d) Cellular oxidative stress, (e) Cellular uptake.

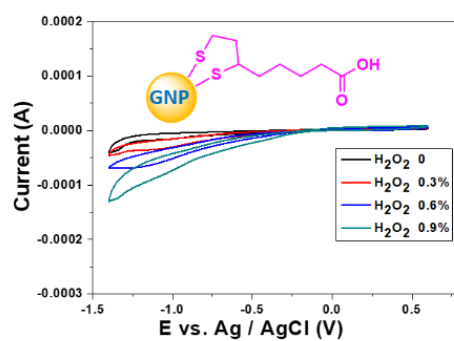
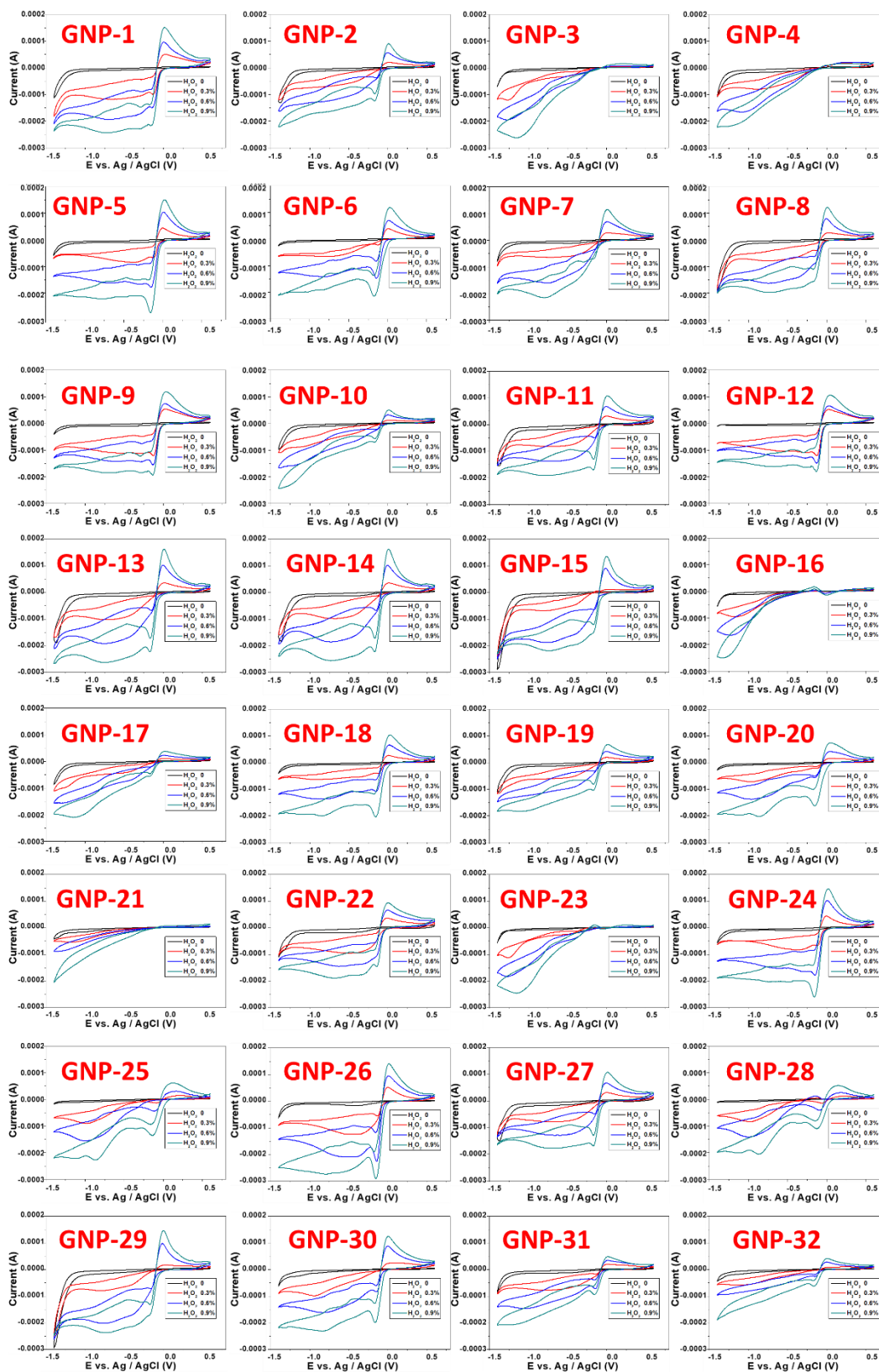
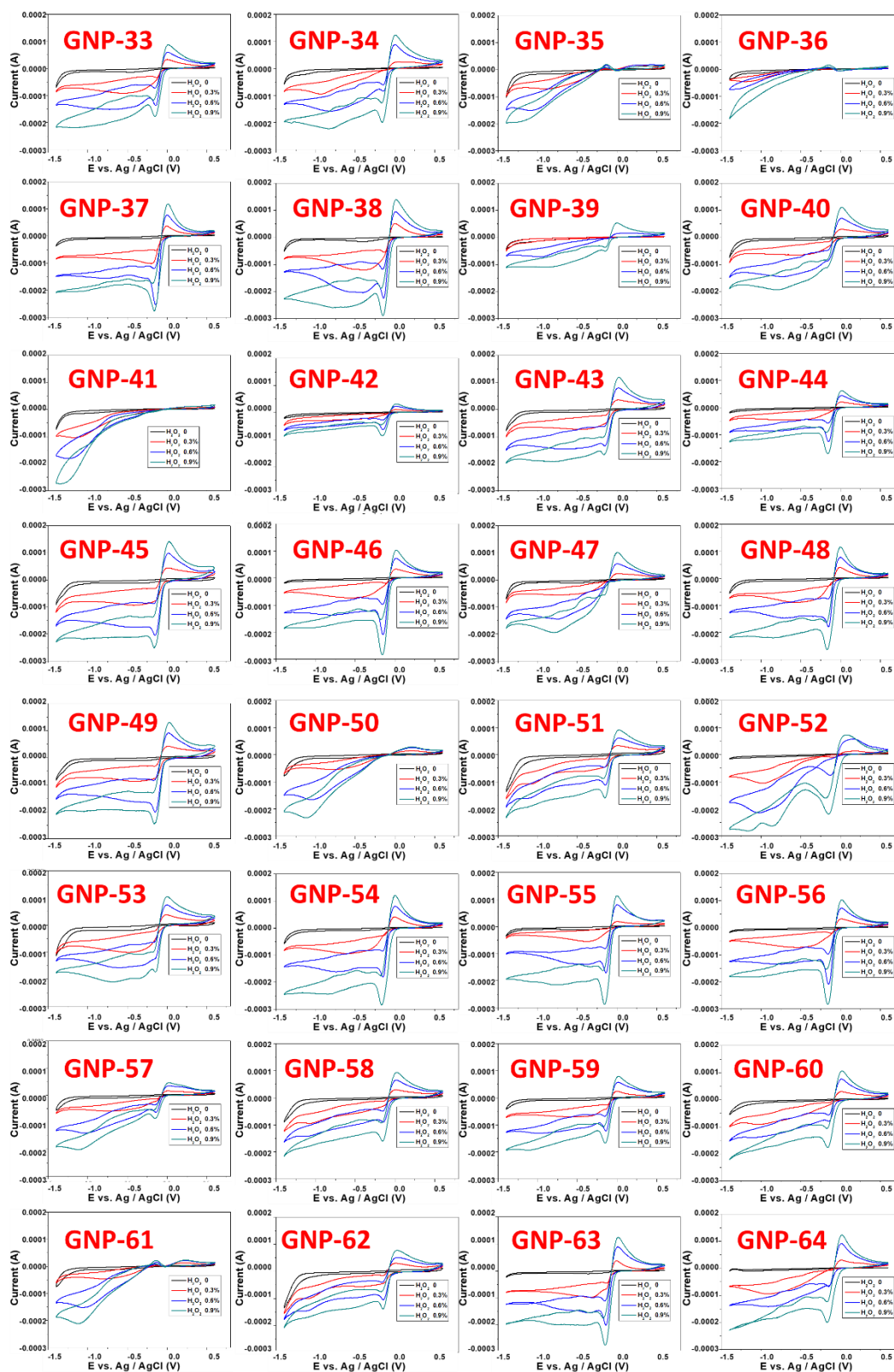


Figure S3. When the ligand does not contain ferrocene substituents, GNPs do not show obvious redox activity. For GNPs, the existence of ferrocene group is a necessary factor to obtain redox activity.







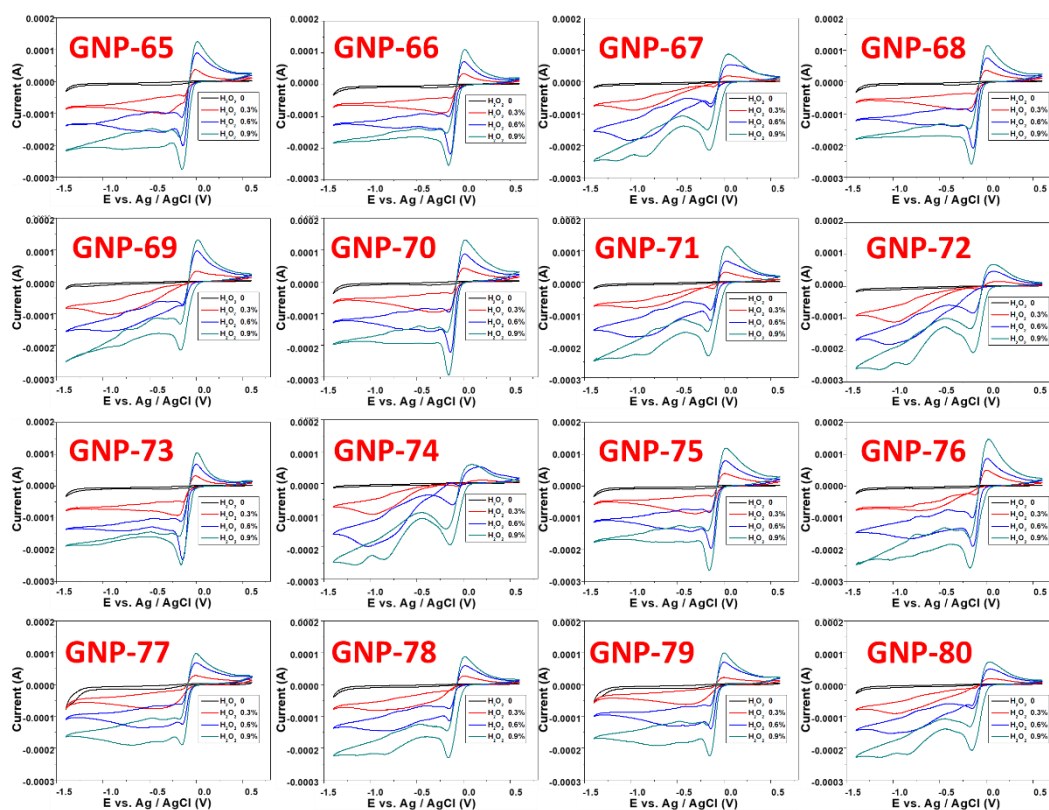
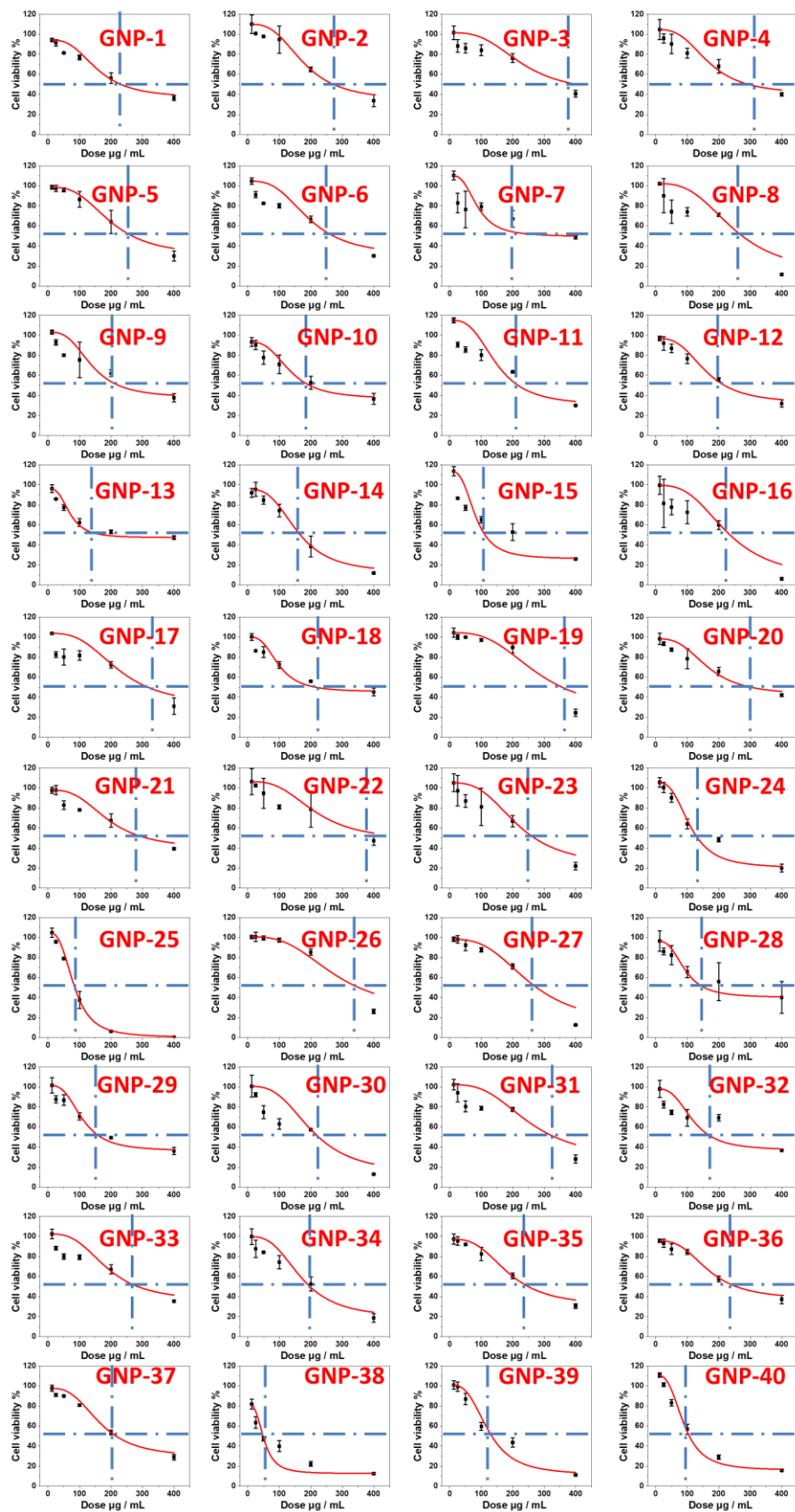


Figure S4. The redox activities of 80 GNPs in the whole library were characterized by cyclic voltammetry.



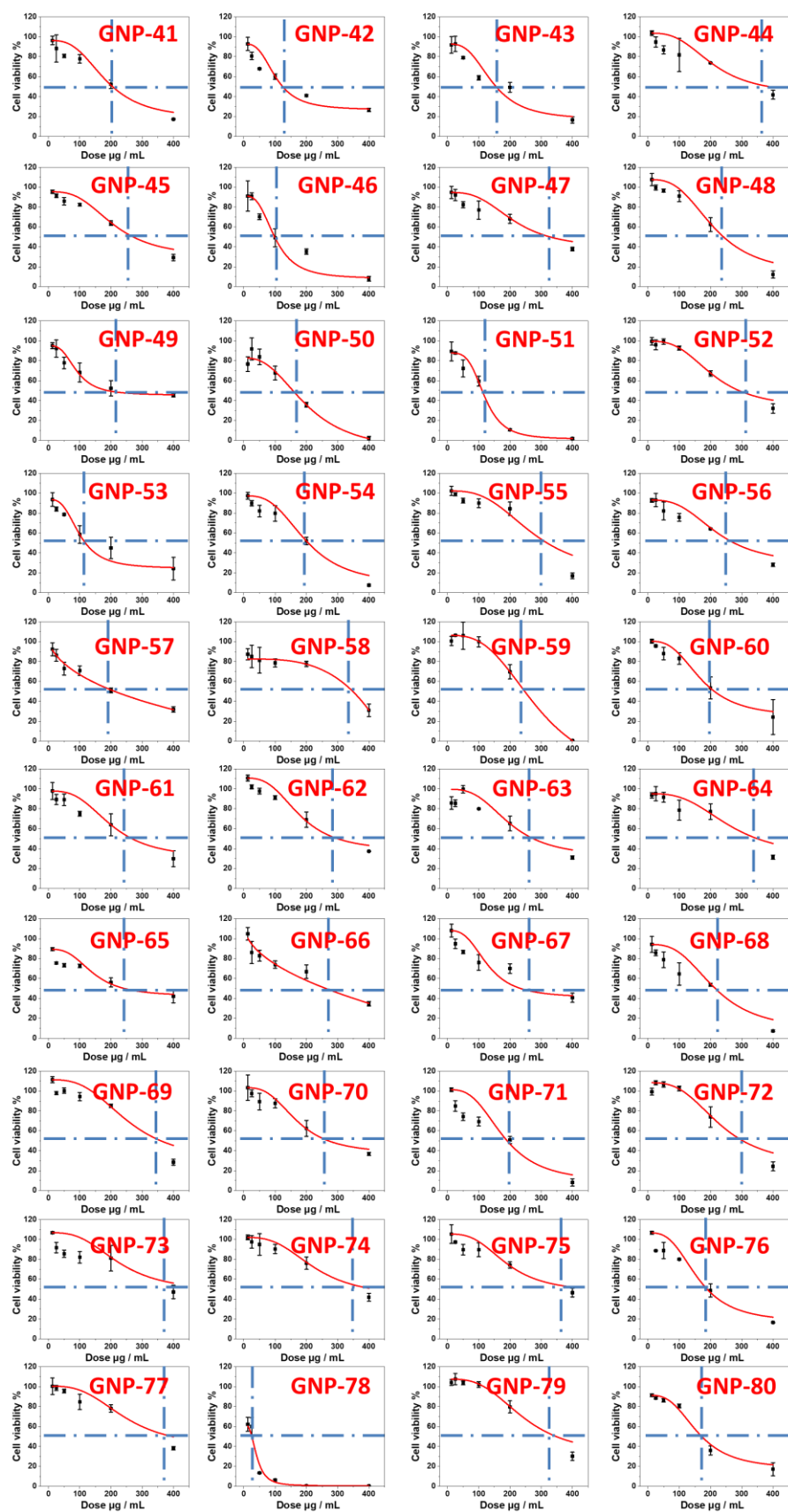


Figure S5. The dose response curves of 80 GNPs in the whole library, blue dotted line:

EC50 labeled.

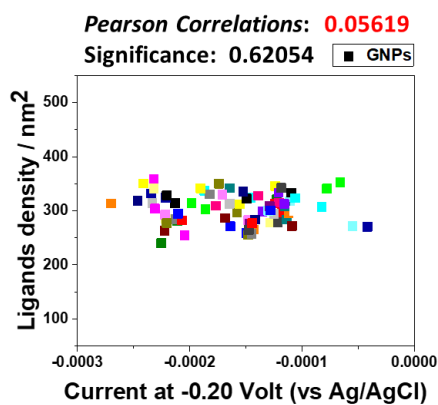


Figure S6. The relationship between the redox activity of 80 GNP<sub>s</sub> and the number of ligand uploads.

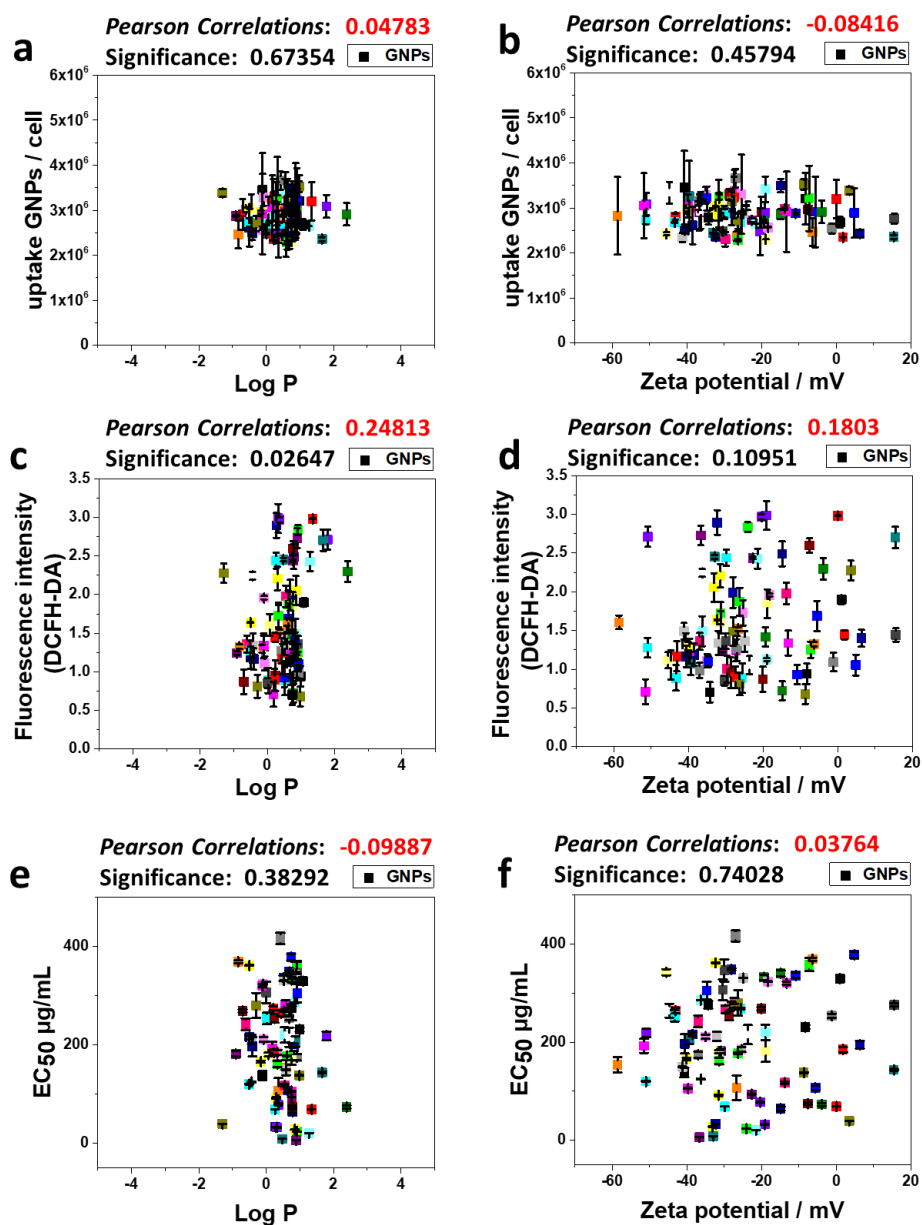


Figure S7. The relationship between the cellular effects of 80 GNPs and hydrophobic properties or surface charge.