Synthesis, Characterization and In-Vitro Anti-Cancer Activity of Vanadium-Doped Nanocrystalline Hydroxyapatite

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Supporting Information

Table S1. Most significant photoelectron scattering paths in the calculated EXAFS of nanocrystalline HAP-V at 295 K.[a]

Path	Legs	Degene-racy	σ^2, Å^2	Length, Å	Contri-bution, %
V0–O4–V0	2	1	0.0006	1.61	100
V0–O3–V0	2	1	0.0010	1.66	84.8
V0–O1–V0	2	1	0.0006	1.99	65.8
V0–O2–V0	2	1	0.0025	2.22	39.4
V0–O14–V0	2	1	0.0043	2.48	26.0
V0–Ca7–V0	2	1	0.0043	2.93	20.2
V0–Ca9–V0	2	1	0.0026	3.23	18.3
V0–Ca8–V0	2	1	0.0010	3.38	18.3
V0–O4–V0–O14-V0	4	2	0.0043	4.10	17.1
V0–Ca10–V0	2	1	0.0043	3.11	17.0
V0–O4–O14–V0	3	2	0.0043	4.09	14.6
V0–Ca11–O3–V0	3	2	0.0011	4.05	12.7
V0–Ca12–V0	2	1	0.0010	3.78	12.4
V0–O3–O4–V0	3	2	0.0016	2.94	12.3
V0–Ca11–V0	2	1	0.0010	3.95	12.0
V0–Ca13–V0	2	1	0.0059	3.60	10.8

[a] The atomic numbering corresponds to Figure 5b (main text). Only the paths with ≥10% contribution are shown. Total of 95 paths (>1% contributions) were used in the calculations. Contributions of the scattering paths were estimated in the FEFF 8.2 theory, taking into account the mean square displacement factors (σ^2) of the atoms.

Table S2. Optimized graphite furnace AAS (Agilent 240Z) parameters for the determination of V content in acidic aqueous solutions and in undiluted cell culture media[a]

Step No.	Temp., K	Time, s	Ar flow, L min^{-1}	Detection
1	358	10	0.3	No
2	368	40	0.3	No
3	393	40	0.3	No
4	673	10[b]	0.3	No
5	1073	10[b]	0.3	No
6	1273	5.0[b]	0.3	No
7	1473	5.0[b]	0.3	No
8	1473	1.0	0.3	Yes
9	1473	2.0	0	Yes
10	2973	1.3	0	Yes
11	2973	2.0	0	Yes
12	2973	2.0	0.3	Yes

[a] The sample volume injected into the furnace was 25 μL. [b] For acidic aqueous solutions (0.10 M HCl), the lengths of these steps could be reduced to 2.0 s without significant effects on the measurement results.

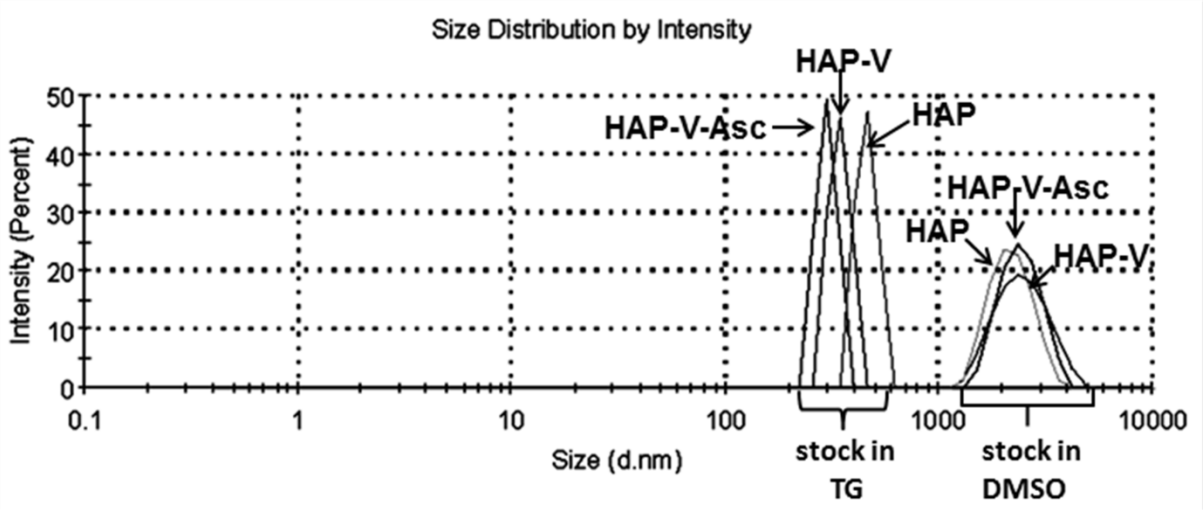
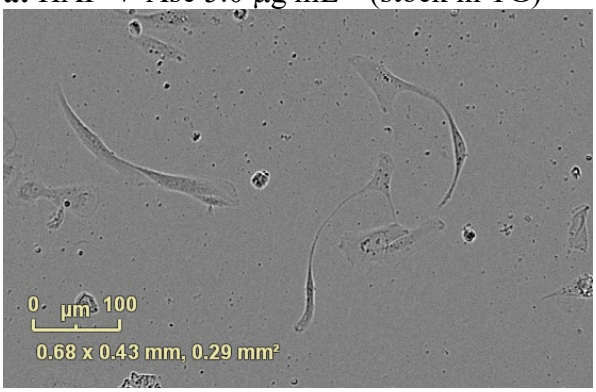
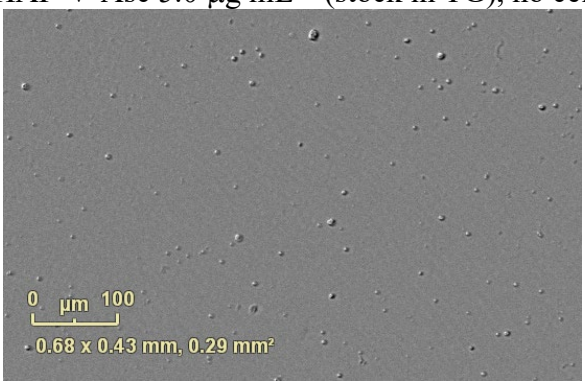


Figure S1. Typical DLS size distribution curves (averages of 10 measurements; 10 s per measurement; 298 K) for suspensions of nanocrystalline HAP (final concentration, 0.25 mg mL^{-1}) in cell culture medium (Advanced DMEM, 2% vol. FCS, 10 mM HEPES, pH 7.4). Designations: HAP is a non-doped sample (black line in Figure 1a, main text); HAP-V is a V-doped sample (red line in Figure 1a); and HAP-V-Asc is HAP-V reduced by 5.0 mM ascorbate at pH = 7.4 (purple lines in Figure 2b,c, main text). Stock suspensions of HAP samples (5.0 mg mL^{-1}) were prepared in either TG or DMSO. Average particle sizes and standard deviations for six replicate measurements are shown in Figure 6a, main text.

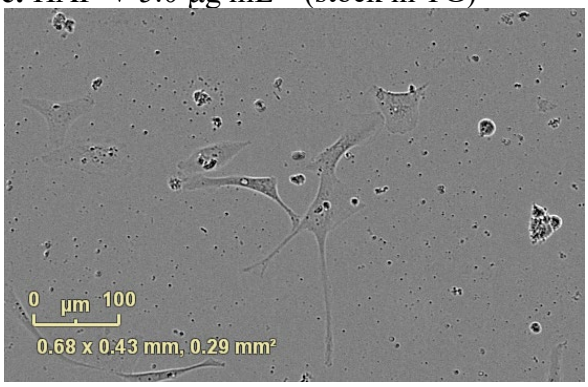
a: HAP-V-Asc 5.0 μg mL^{-1} (stock in TG)



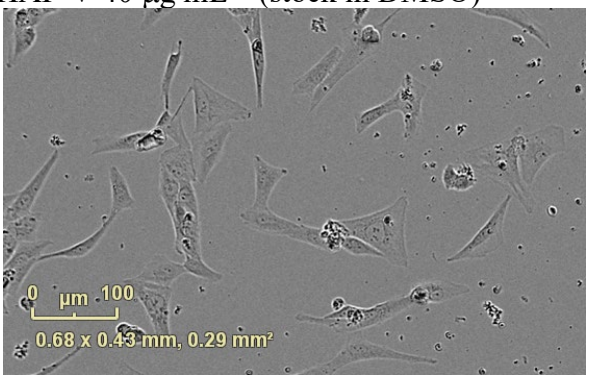
b: HAP-V-Asc 5.0 μg mL^{-1} (stock in TG), no cells



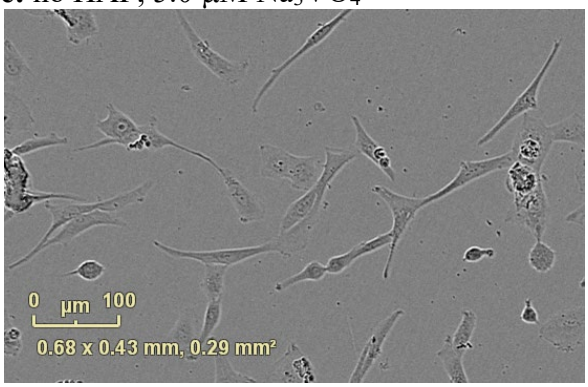
c: HAP-V 5.0 μg mL^{-1} (stock in TG)



d: HAP-V 40 μg mL^{-1} (stock in DMSO)



e: no HAP, 5.0 μM Na_3VO_4



f: no additions

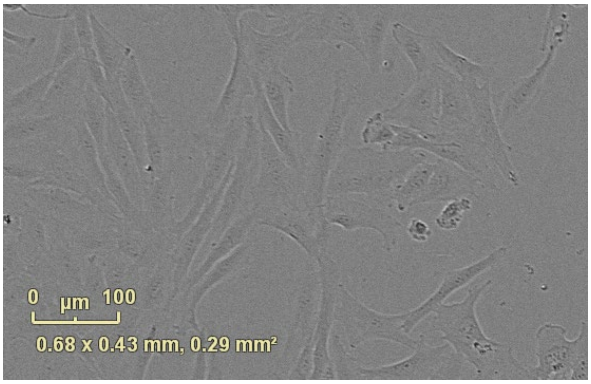


Figure S2. Typical phase contrast light microscope (IncuCyte Zoom; x10 objective) views of SW1353 cells after incubation in the presence or absence of HAP particles for 72 h.