Supplementary information

Effect of water-soluble chlorine-containing buckminsterfullerene derivative on the metabolism of reactive oxygen species in human embryonic lung fibroblasts

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Synthesis of compound F1

Water-soluble fullerene derivative **F1** (scheme S1) was synthesized in three synthetic steps and characterized as reported before [1].

First, chlorofullerene $C_{60}Cl_6$ obtained as described previously [2] was arylated with the excess of dimethyl ester of 3-phenylglutaric acid to obtain fullerene derivative **1** [1]. Compound **1** was purified using preparative HPLC, then ester groups in its structure were hydrolyzed to obtain fullerene-based acid **2** [1]. Synthesized acid was solubilized in water containing 2.5 eq of K_2CO_3. Obtained solution was filtered and then lyophilized to provide water-soluble salt **F1**.

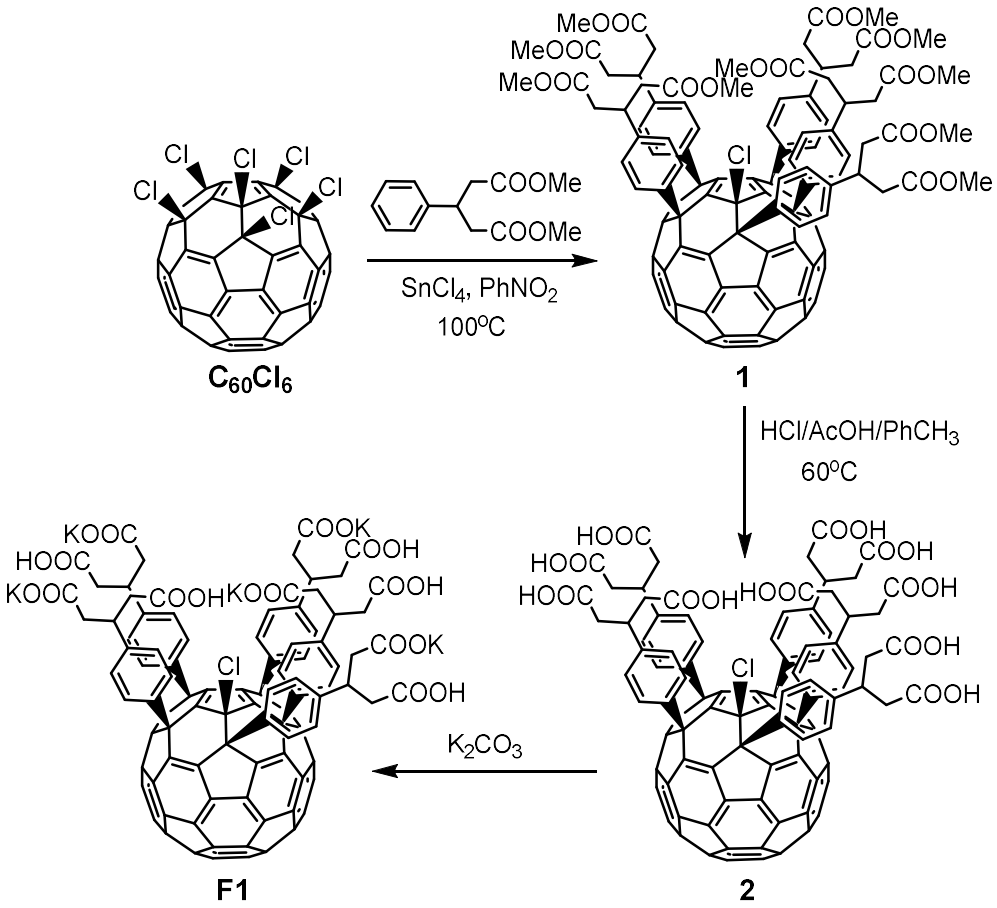


Figure S1. Synthesis of water-soluble fullerene derivative F1 from chlorofullerene $C_{60}Cl_6$.

Dynamic light scattering measurements

As most of the amphiphilic fullerene derivatives, water-soluble compound F1 forms bilayer vesicles with average hydrodynamic radius <Rh> = 50 nm in aqueous solution.

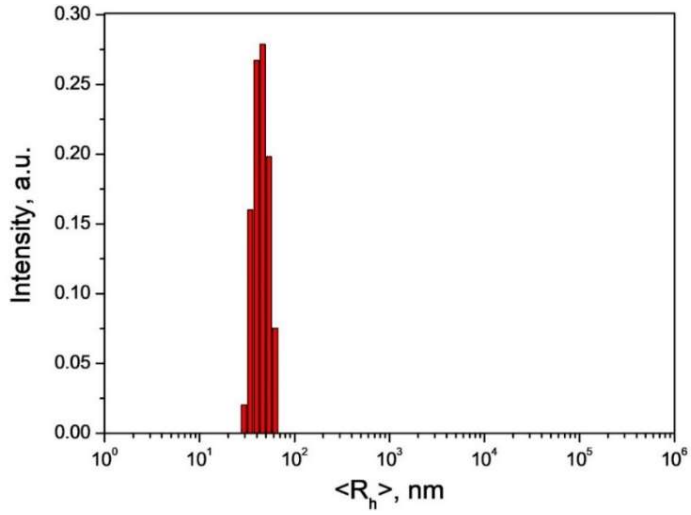


Figure S2. DLS profile revealing particle size distribution in aqueous solutions of the fullerene derivative **F1**.

The fluorescence and absorption spectra of the fullerene derivative

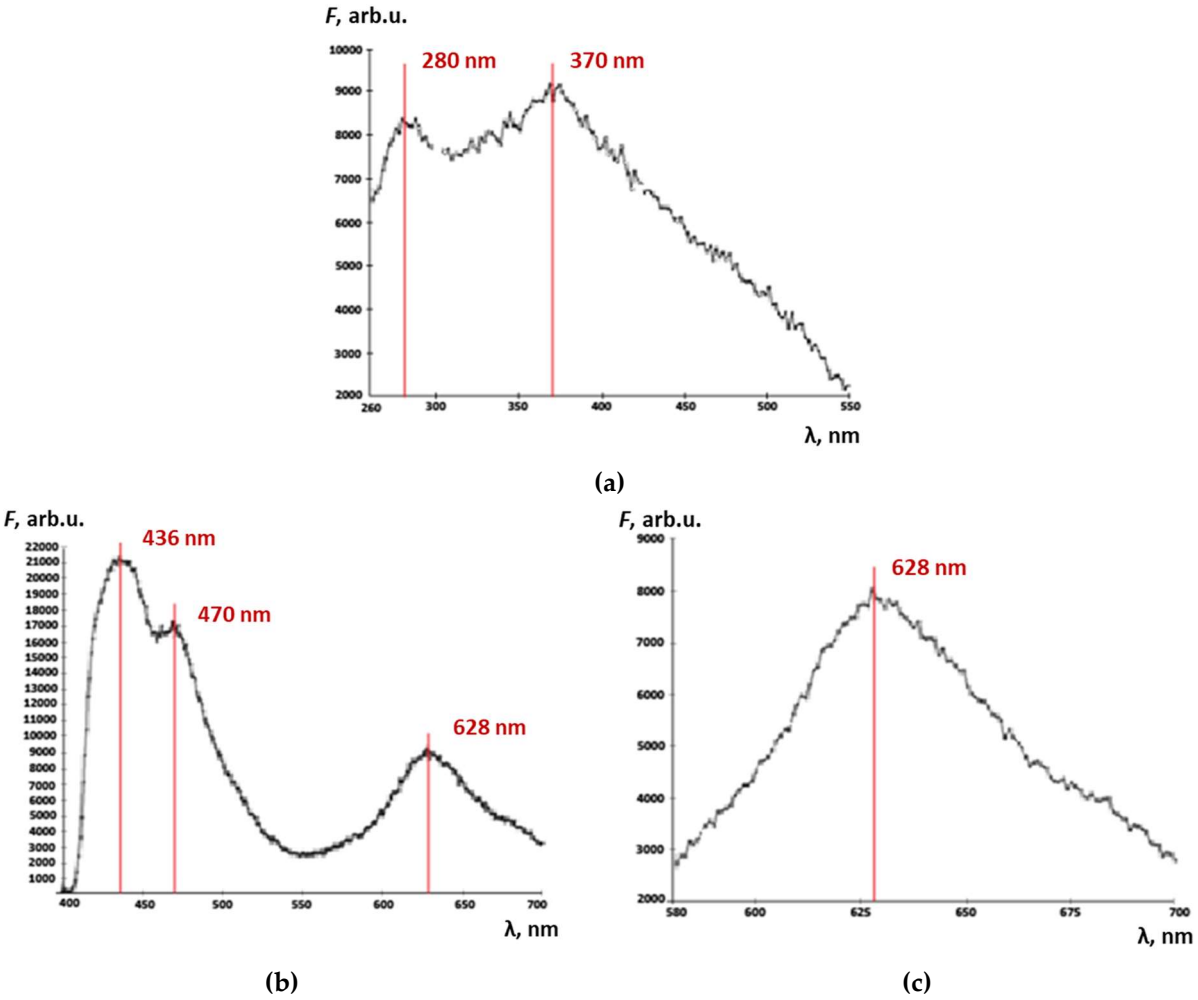


Figure S3. The excitation spectrum of the **F1** solution in the culture medium (1.5 μM) (λ_{fl} = 620 nm) (a); the fluorescence spectra of **F1** at λ_{ex} = 280 nm (b) and λ_{ex} = 370 nm (c).

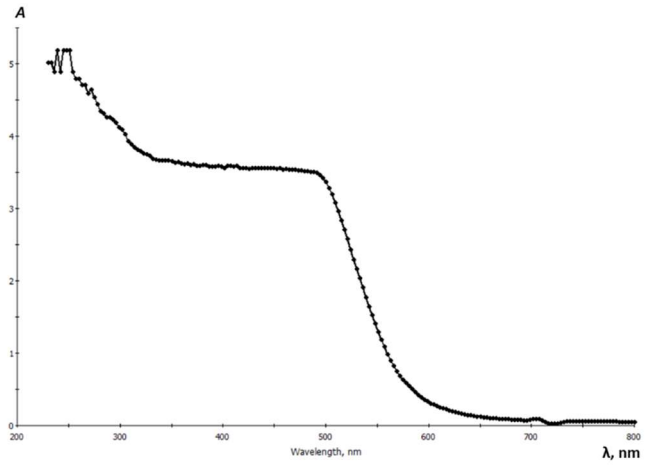
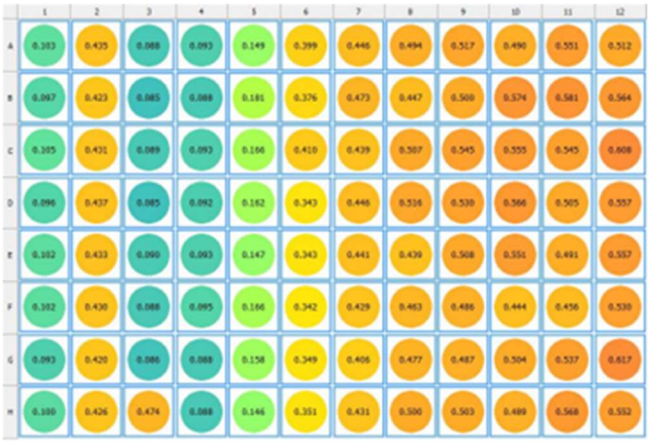
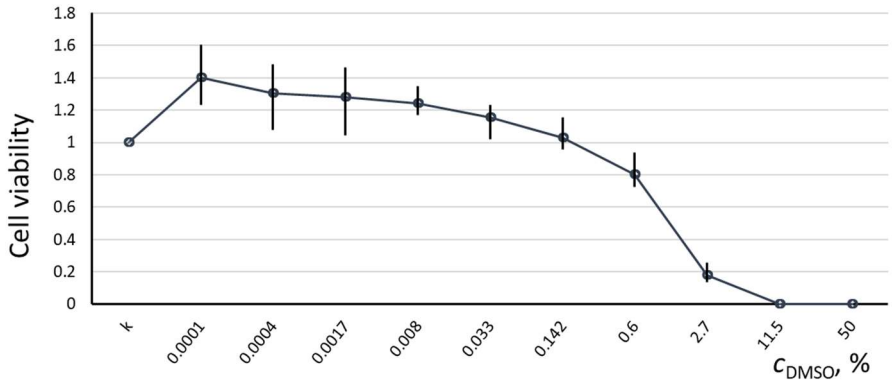


Figure S4. The absorption spectrum of the **F1** solution in deionized water (1.5 μM).

MTT-test, the positive control with dimethyl sulfoxide



(a)



(b)

Figure S5. MTT-test: the positive control with dimethyl sulfoxide (0.0001%–50%); a 96-well scheme (a) and the cell viability *vs* DMSO concentration (b).

References

1 Kraevaya, O.A.; Peregudov, A.S.; Troyanov, S.I.; Godovikov, I.; Fedorova, N.E.; Klimova, R.R.; Sergeeva, V.A.; Kameneva, L.V.; Ershova, E.S.; Martynenko, V.M., et al. Diversion of the Arbuzov reaction: alkylation of C-Cl instead of phosphonic ester formation on the fullerene cage. *Org Biomol Chem* **2019**, 17, 7155-7160, doi:10.1039/c9ob00593e.

2 Troshin, P.A.; Popkov, O.; Lyubovskaya R.N. Some New Aspects of Chlorination of Fullerenes. *Fullerenes, Nanotubes, Carbon Nanostruct*. **2003**, 11, 165-185, doi: 10.1081/FST-120021142.