Electronic supplementary information for the manuscript

«Influence of water-soluble derivatives of [60]fullerene on therapeutically important targets related to neurodegenerative diseases»

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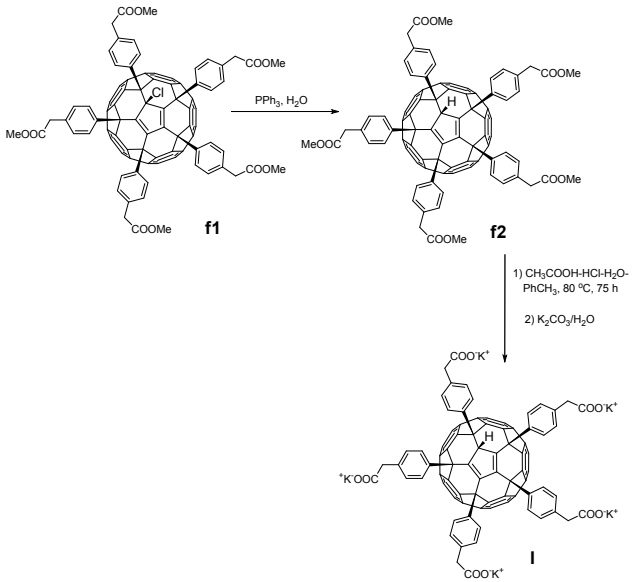
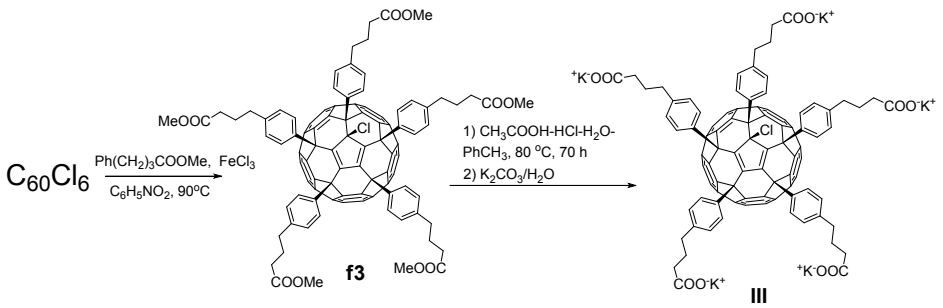
Compound **I** has been synthesized in two steps according to the scheme 1. Preparation and spectral properties of the chlorine-containing precursor **f1** are described previously (O. A. Troshina, P. A. Troshin, A. S. Peregudov, V. I. Kozlovskiy, J. Balzarini and R. N. Lyubovskaya, *Org. Biomol. Chem*, 2007, **5**, 2783–2791.).



Scheme 1

Compound **II**, which was a mixture of metallated hydroxyfullerenes with narrow molecular weight distribution ("potassium fullerenolate") was prepared according to the method reported previously (P. A.Troshin, A. S. Astakhova and R. N. Lyubovskaya, *Fuller. Nanotub. Carb. Nanostruct.*, 2005, **13**, 331-343.). The data on the composition of **II** and its chemical nature and some biological properties were presented previously (A. G. Bobylev, A. B. Kornev, L. G. Bobyleva, M. D. Shpagina, I. S. Fadeeva, R. S. Fadeev, D. G. Deryabin, J. Balzarini, P. A. Troshin and Z. A. Podlubnaya, *Org. Biomol. Chem*, 2011, **9**, 5714-5719).
Compound **III** has been synthesized in two steps from $C_{60}Cl_6$ according to the scheme 2.



Scheme 2

The compositions and structures of intermediate products **f2**, **f3** and compounds **I** and **III** (in the form of free acids) has been confirmed using ^1H and ^{13}C NMR spectroscopy in combination with ESI mass spectrometry.
*Spectral characteristics of **f2**:* ^1H NMR (600 MHz, $CDCl_3$, δ, ppm): 3.40-3.80 (m, 25H), 5.25 (s, 1H), 7.09 (d, 2H), 7.13 (d, 4H), 7.27 (d, 4H), 7.37 (d, 2H), 7.55 (d, 4H), 7.73 (d, H). ^{13}C NMR (150 MHz, $CDCl_3$, δ, ppm): 40.65 (CH_2), 40.78 (CH_2),

40.85 (*C*H_2), 52.01 (O*C*H_3), 52.10 (O*C*H_3), 52.15 (O*C*H_3), 58.58 (sp^3, cage), 58.69 (sp^3, cage), 60.71 (sp^3, cage), 62.82 (sp^3, cage), 127.96 (Ar), 128.24 (Ar), 128.38 (Ar), 129.61 (Ar), 129.75 (Ar), 129.88 (Ar), 133.02, 133.39, 133.64, 138.60, 143.19, 143.71, 144.10, 144.18, 144.28, 144.36, 144.39, 144.49, 145.35, 145.60, 145.82, 145.93, 146.05, 146.92, 147.11, 147.21, 147.68, 147.76, 148.11, 148.28, 148.41, 148.71, 148.74, 148.79, 151.52, 152.08, 152.60, 156.03, 171.74 (*C*$OOCH_3$), 171.79 (*C*$OOCH_3$), 171.81 (*C*$OOCH_3$).

Spectral characteristics of ***f3***: ^{1}H NMR (600 MHz, $CDCl_3$, δ, ppm): 1.56 (m, 4H), 1.67 (m, 16H), 2.26 (t, 2H), 2.34 (t, 8H), 2.51 (t, 2H), 2.65 (t, 8H), 3.60 (s, 3H), 3.64 (s, 6H), 3.65 (s, 6H), 6.90 (d, 2H), 7.06 (d, 4H), 7.13 (d, 4H), 7.14 (d, 2H), 7.53 (d, 4H), 7.81 (d, 4H). ^{13}C NMR (150 MHz, $CDCl_3$, δ, ppm): 24.47 (*C*H_2), 24.61 (*C*H_2), 24.64 (*C*H_2), 30.58 (*C*H_2), 30.70 (*C*H_2), 30.82 (*C*H_2), 33.88 (*C*H_2), 33.91 (*C*H_2), 33.93 (*C*H_2), 35.11 (*C*H_2), 35.14 (*C*H_2), 35.20 (*C*H_2), 51.48 (O*C*H_3), 51.52 (O*C*H_3), 58.00 (sp^3, cage), 60.61 (sp^3, cage), 63.26 (sp^3, cage), 76.38 (*C*-Cl), 127.79, 128.61, 128.64, 128.70, 128.75, 128.77, 128.79, 128.83, 130.20, 134.93, 136.44, 141.19, 141.48, 141.72, 141.75, 142.88, 143.49, 143.71, 143.84, 143.86, 144.15, 144.17, 144.29, 144.41, 144.55, 145.40, 145.48, 146.94, 147.29, 147.32, 147.45, 147.90, 148.16, 148.31, 148.50, 148.66, 148.70, 148.72, 148.82, 150.59, 151.37, 153.79, 156.88, 173.98 (*C*$OOCH_3$), 174.02 (*C*$OOCH_3$), 174.04 (*C*$OOCH_3$).

Spectral characteristics of ***I***: . ^{1}H NMR (600 MHz, CS_2+acetone-D_6, δ, ppm): 3.45-3.70 (m, 10H), 5.45 (s, 1H), 7.06 (d, 2H), 7.16 (d, 4H), 7.30 (d, 4H), 7.33 (d, 2H). 7.58 (d, 4H), 7.80 (d, 4H). ^{13}C NMR (150 MHz, CS_2+acetone-D_6, δ, ppm): 40.25 (*C*H_2), 40.34 (*C*H_2), 40.39 (*C*H_2), 58.64 (sp^3, cage), 58.82 (sp^3, cage), 60.83 (sp^3, cage), 63.02 (sp^3, cage), 127.74 (Ar), 128.15 (Ar), 128.28 (Ar), 129.85 (Ar), 129.98 (Ar), 130.14 (Ar), 130.24 (Ar), 130.27 (Ar), 134.40, 137.77, 143.27, 144.07, 144.18, 144.25, 144.34, 144.48, 144.79, 145.65, 145.91, 146.11, 146.97, 147.18, 147.28, 147.80, 148.13, 148.32, 148.45, 148.73, 148.79, 151.95, 152.64, 156.61, 170.81 (*C*OOH), 171.54 (*C*OOH), 171.82 (*C*OOH).

Spectral characteristics of ***III*****:** ^{1}H NMR (600 MHz, CS_2+acetone-D_6, δ, ppm): 1.59 (m, 4H), 1.69 (m, 16H), 2.27 (t, 2H), 2.35 (m, 8H), 2.55 (t, 2H), 2.70 (m, 8H), 6.95 (d, 2H), 7.15 (d, 2H), 7.16 (d, 4H), 7.23 (d, 4H), 7.57 (d, 4H), 7.85 (d, 4H). ^{13}C NMR (150 MHz, CS_2+acetone-D_6, δ, ppm): 24.60 (*C*H_2), 24.72 (*C*H_2), 24.84 (*C*H_2), 30.93 (*C*H_2), 30.95 (*C*H_2), 31.01 (*C*H_2), 33.41 (*C*H_2), 33.51 (*C*H_2), 33.53 (*C*H_2), 35.23 (*C*H_2), 35.31 (*C*H_2), 35.39 (*C*H_2), 58.00 (sp^3, cage), 60.68 (sp^3, cage), 63.28 (sp^3, cage), 76.59 (*C*-Cl), 128.01 (Ar), 128.60 (Ar), 128.74 (Ar), 129.04 (Ar), 130.23 (Ar), 134.46, 135.97, 141.03, 141.68, 142.14, 142.19, 142.97, 143.63, 143.83, 143.94, 143.98, 144.26, 144.27, 144.37, 144.44, 144.64, 145.51, 145.62, 147.12, 147.32, 147.35, 147.48, 147.92, 148.17, 148.33, 148.53, 148.67, 148.73, 148.83, 150.74, 151.51, 153.75, 156.98, 174.37 (*C*OOH), 174.39 (*C*OOH), 174.45 (*C*OOH).