

**Carboxylic fullerene C<sub>60</sub> derivatives: efficient microbicides against herpes simplex virus and cytomegalovirus infections *in vitro***

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*Synthesis of compound 3.* Chlorofullerene C<sub>60</sub>Cl<sub>6</sub> (1 g) and 300 ml of dried and freshly distilled nitrobenzene were introduced into a three-necked 500 ml round-bottom flask equipped with a reversed condenser and a thermometer and filled with argon. The mixture was stirred under argon until complete dissolving of C<sub>60</sub>Cl<sub>6</sub> was observed. The introduction of 30 ml of methyl 4-biphenylacetate was followed by addition of a small amount of anhydrous FeCl<sub>3</sub> (20–30 mg). The reaction mixture was heated to 90–110 °C under continuous stirring within 20–40 min until complete disappearance of starting C<sub>60</sub>Cl<sub>6</sub> as followed by TLC. The reaction mixture was cooled down to the room temperature and washed with diluted HCl (ca. 1%) and deionized water, dried over MgSO<sub>4</sub>, diluted with hexanes and subjected to column chromatography separation on silica gel. Compound **3** in the form of methyl ester (860 mg, 43%) was obtained by elution with a toluene–methanol (99.5 : 0.5 v/v) mixture. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz): 3.63–3.77 (m, 25H), 7.29 (d, 2H), 7.38–7.41 (m, 12H), 7.48–7.51 (d, 2H), 7.56–7.59 (d, 4H), 7.59–7.62 (d, 4H), 7.62–7.67 (m, 8H), 7.81–7.85 (d, 4H), 8.09–8.12 (d, 4H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz): 40.82 (CH<sub>2</sub>), 40.85 (CH<sub>2</sub>), 40.87 (CH<sub>2</sub>), 52.12 (OCH<sub>3</sub>), 52.19 (OCH<sub>3</sub>), 58.06 (sp<sup>3</sup> cage), 60.66 (sp<sup>3</sup> cage), 63.31 (sp<sup>3</sup> cage), 76.35 (C–Cl), 126.50, 127.23, 127.34, 127.43, 127.46, 128.26, 129.07, 129.09, 129.62, 129.81, 129.86, 130.58, 133.18, 133.34, 133.37, 136.41, 137.89, 138.91, 139.16, 139.21, 139.61, 140.31, 140.35, 142.76, 143.05, 143.40, 143.55, 143.79, 143.94, 144.07, 144.33, 144.43, 144.56, 144.69, 145.35, 145.44, 146.76, 147.35, 147.47, 147.96, 148.25, 148.40, 148.58, 148.77, 148.82, 148.88, 150.38, 151.27, 153.92, 156.72, 171.96 (COOCH<sub>3</sub>), 172.01 (COOCH<sub>3</sub>). The aforementioned fullerene derivative (500 mg) was dissolved in toluene (100 ml) and then 300 ml of glacial acetic acid and 50 ml of 36% aqueous HCl were added. The resulting two-phase mixture was heated at 60–70 °C for 36 h, then the solvents were removed at the rotary evaporator and the solid residue was washed with diethyl ether and dried in vacuum. This procedure yielded 440 mg (91%) of compound **3** in the form of free acid. <sup>1</sup>H NMR [CS<sub>2</sub>-(CD<sub>3</sub>)<sub>2</sub>CO, 600 MHz]: 3.55 (s, 2H), 3.61 (s, 8H), 7.27 (d, 2H), 7.35 (m, 8H), 7.44 (d, 2H), 7.55

(d, 4H), 7.59 (d, 4H), 7.62 (d, 4H), 7.70 (d, 4H), 7.84 (d, 4H), 8.12 (d, 4H).  $^{13}\text{C}$  NMR [ $\text{CS}_2$ - $(\text{CD}_3)_2\text{CO}$ , 150 MHz]: 40.37 ( $\text{CH}_2$ ), 40.44 ( $\text{CH}_2$ ), 58.05 ( $\text{sp}^3$  cage), 60.73 ( $\text{sp}^3$  cage), 63.38 ( $\text{sp}^3$  cage), 76.49 (C-Cl), 126.62, 126.97, 127.08, 127.54, 127.59, 129.11, 129.24, 129.95, 130.06, 130.07, 130.75, 134.24, 134.33, 134.38, 135.95, 137.35, 138.47, 138.56, 138.63, 139.93, 140.62, 140.70, 142.42, 143.15, 143.62, 143.73, 143.92, 143.94, 144.20, 144.42, 144.53, 144.61, 144.79, 145.51, 145.59, 146.94, 147.38, 147.41, 147.54, 148.02, 148.28, 148.43, 148.63, 148.79, 148.83, 148.85, 148.94, 150.61, 151.35, 153.96, 156.92, 171.42 (COOH), 171.49 (COOH), 171.53 (COOH).