

Electronic supplementary information (ESI)  
for

**Hybrid photoactive fullerene derivative – ruboxyl nanostructures for photodynamic therapy**

Alexander I. Kotelnikov<sup>a\*</sup>, Alexander Yu. Rybkin<sup>a</sup>, Ekaterina A. Khakina<sup>a</sup>, Alexey B. Kornev<sup>a</sup>, Alexander V. Barinov<sup>a</sup>, Nikolay S. Goryachev<sup>a</sup>, Anastasiya V. Ivanchikhina<sup>a</sup>, Alexander S. Peregudov<sup>b</sup>, Vyacheslav M. Martynenko<sup>a</sup> and Pavel A. Troshin<sup>a</sup>

<sup>a</sup> IPCP RAS, Semenov Prospect 1, Chernogolovka, 141432, Russia. Fax: +7 496522-3507; Tel: +7 496522 1418; E-mails: [kotel@icp.ac.ru](mailto:kotel@icp.ac.ru), [troshin@icp.ac.ru](mailto:troshin@icp.ac.ru).

<sup>b</sup> INEOS RAS, Vavylova St. 28, B-334, Moscow, 119991, Russia

Table of contents

**Fig. 1S.** The IR spectra of the fullerene derivative **1 (a)**, ruboxyl **3 (b)** and the conjugate **4 (c)**.

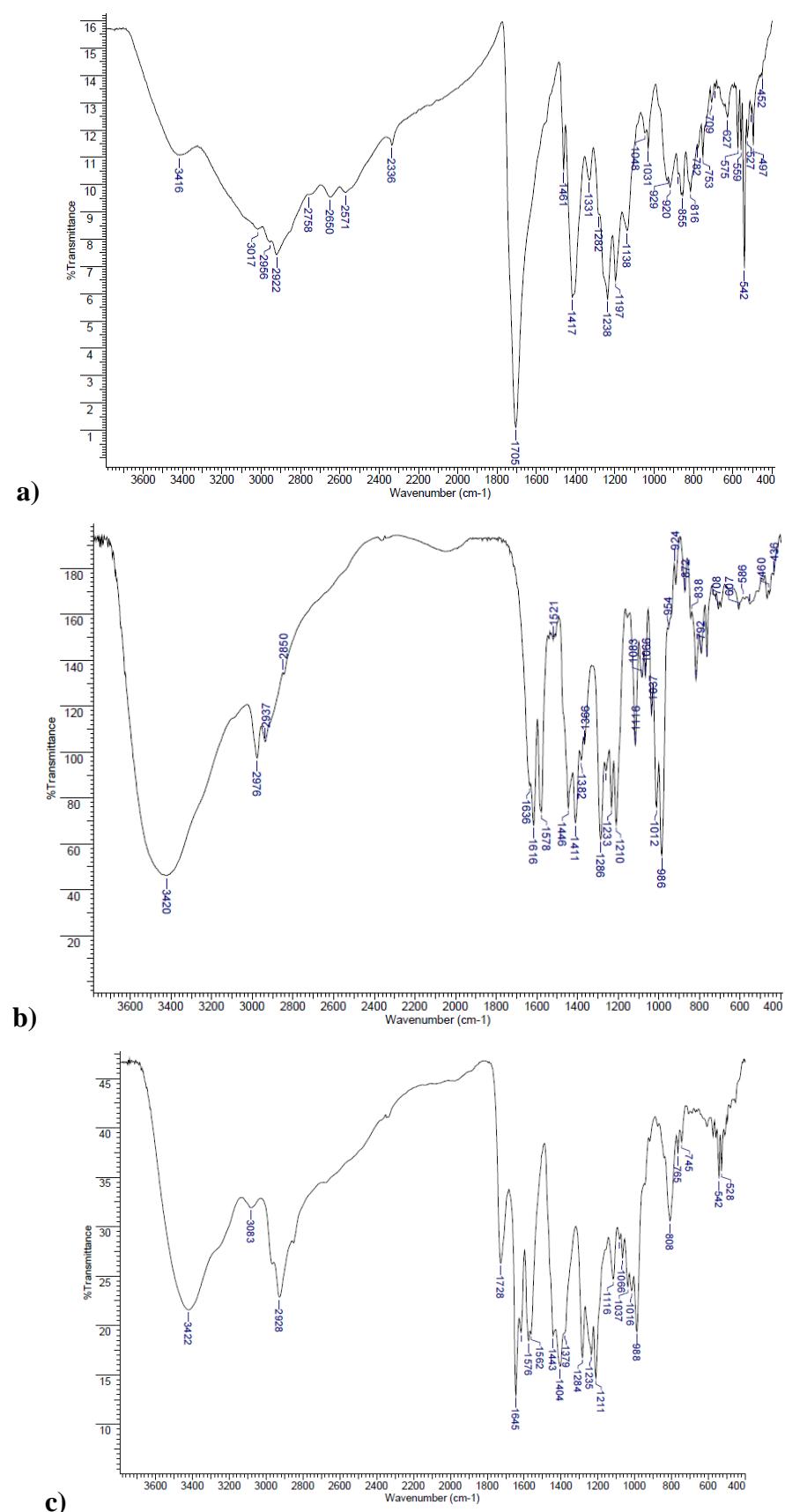
**Fig. S2.** The <sup>1</sup>H (a) and <sup>13</sup>C NMR (b) spectra of the fullerene-ruboxyl conjugate **4**. Groups of the signals marked with “\*” correspond to the fullerene moiety bearing SCH<sub>2</sub>CH<sub>2</sub>COOR groups.

**Fig. S3.** The <sup>1</sup>H (a) and <sup>13</sup>C NMR (b) spectra of the fullerene-ruboxyl conjugate **5**. Symbol “\*\*” denotes solvent peaks.

**Fig. S4.** The H-H COSY NMR spectrum of the fullerene-ruboxyl conjugate **5**.

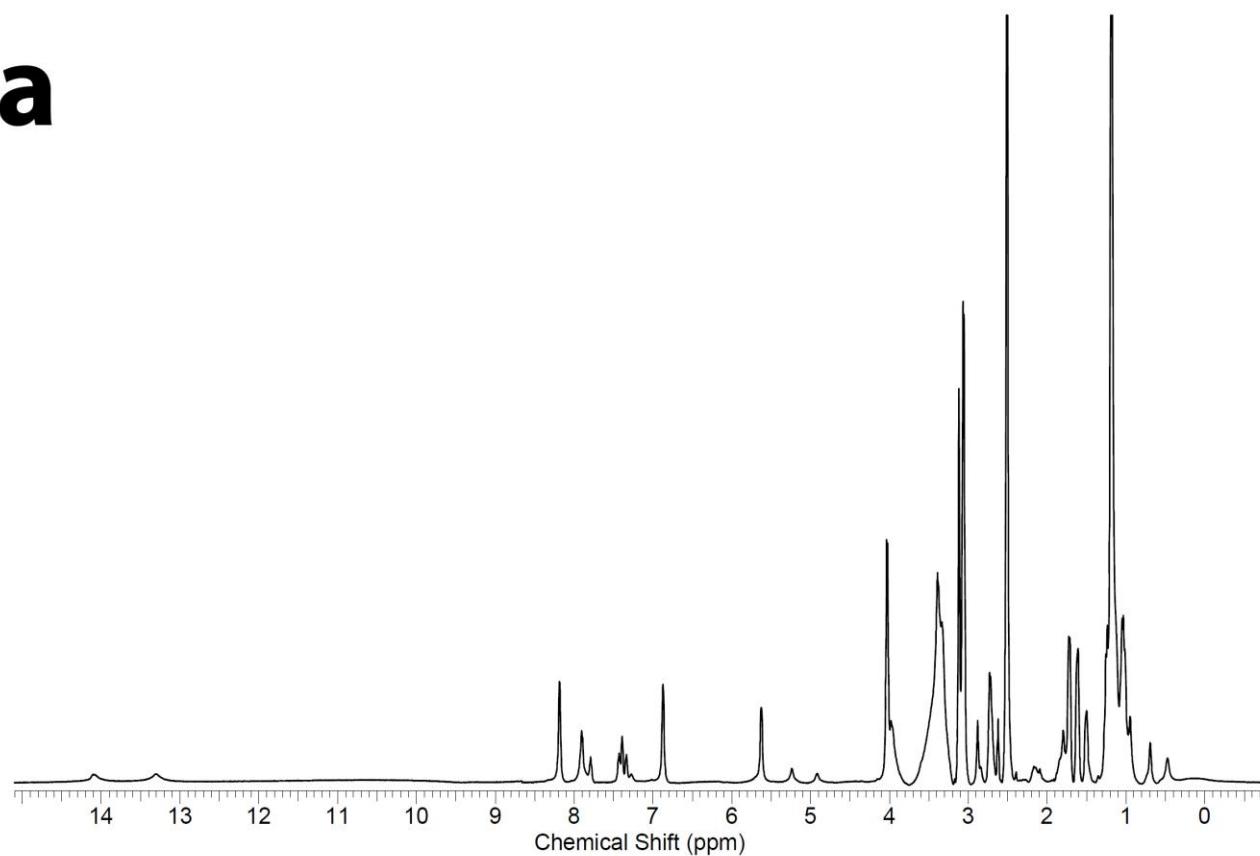
**Fig. S5.** The H-C HMBC NMR spectrum of the fullerene-ruboxyl conjugate **5**.

**Fig. S6.** ESI mass-spectrum of conjugate **5**

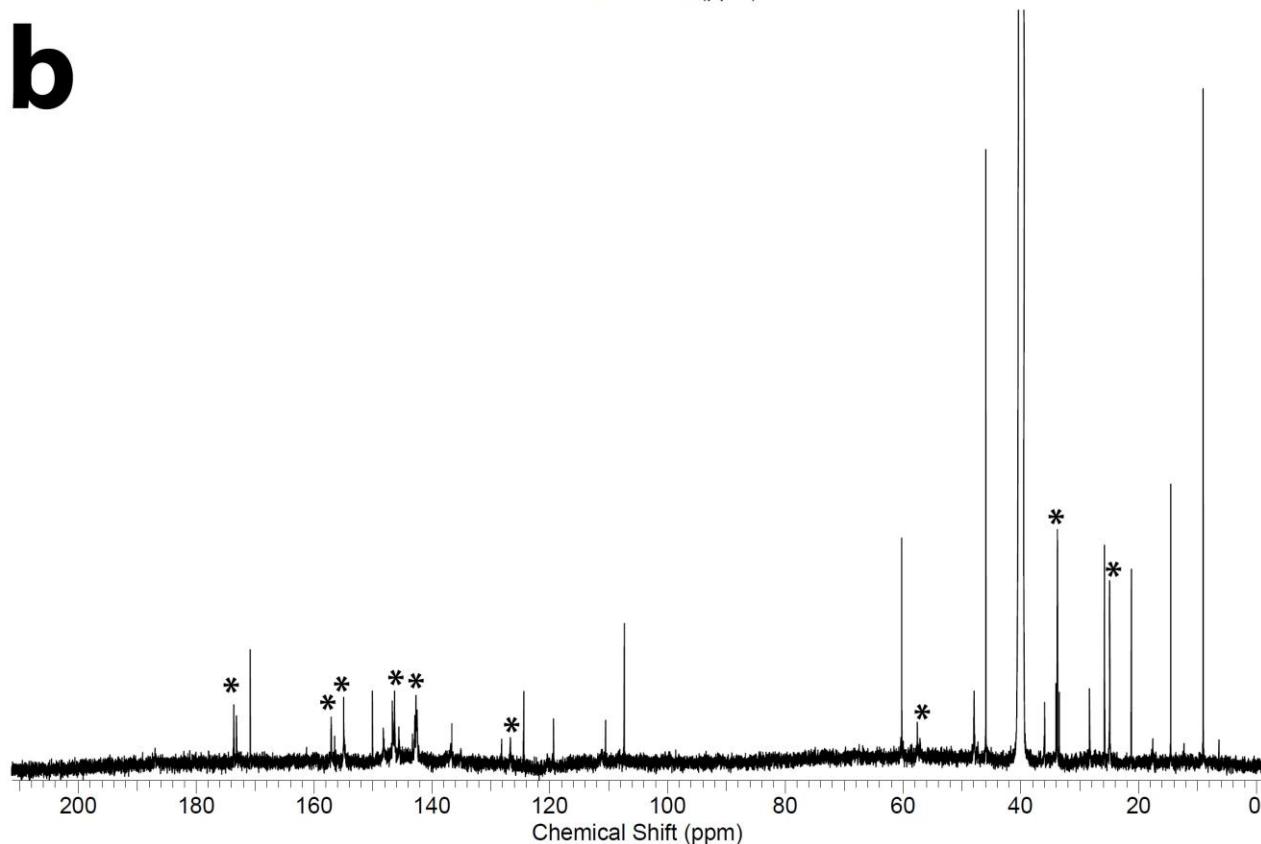


**Fig. 1S.** The IR spectra of the fullerene derivative **1** (a), rubroxyl **3** (b) and the conjugate **4** (c).

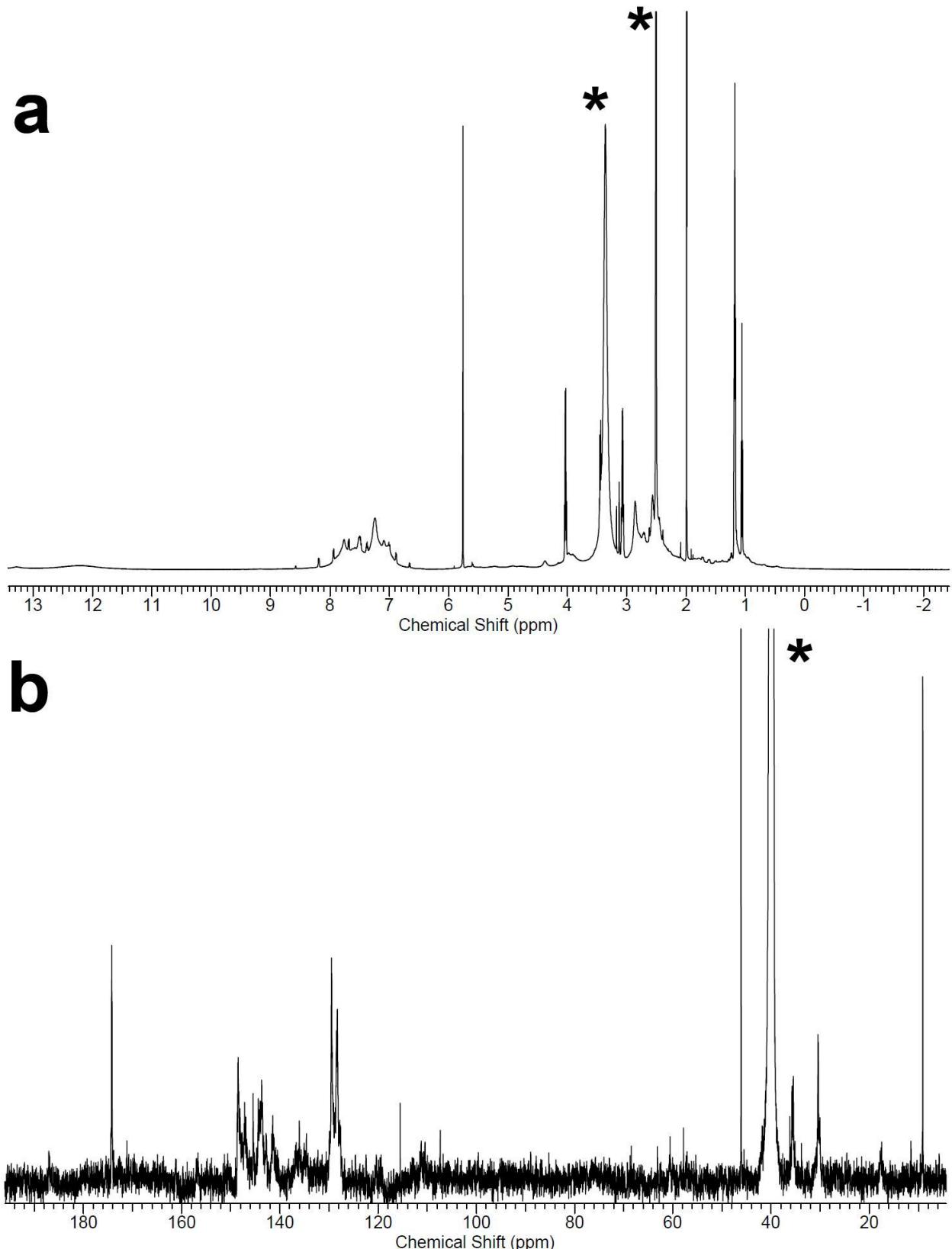
a



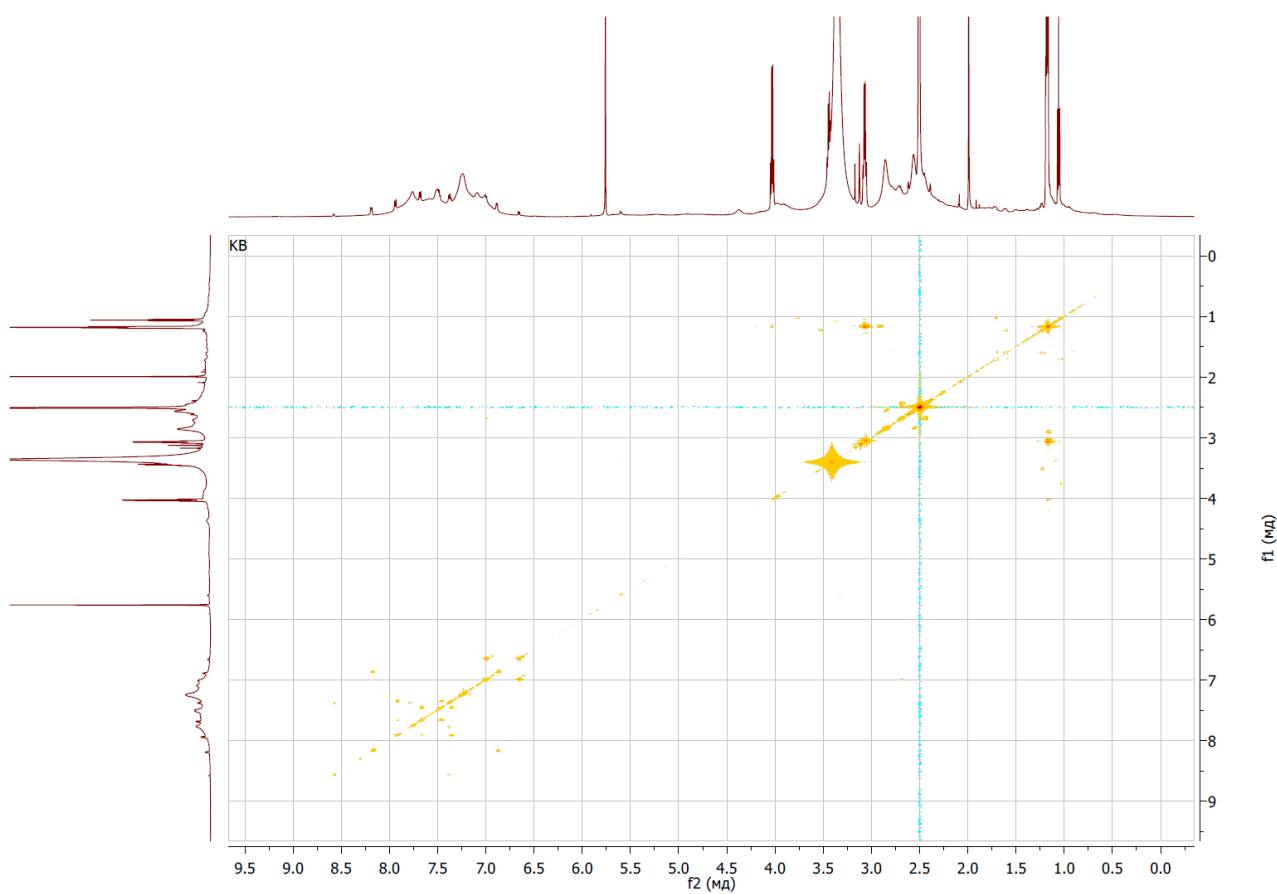
b



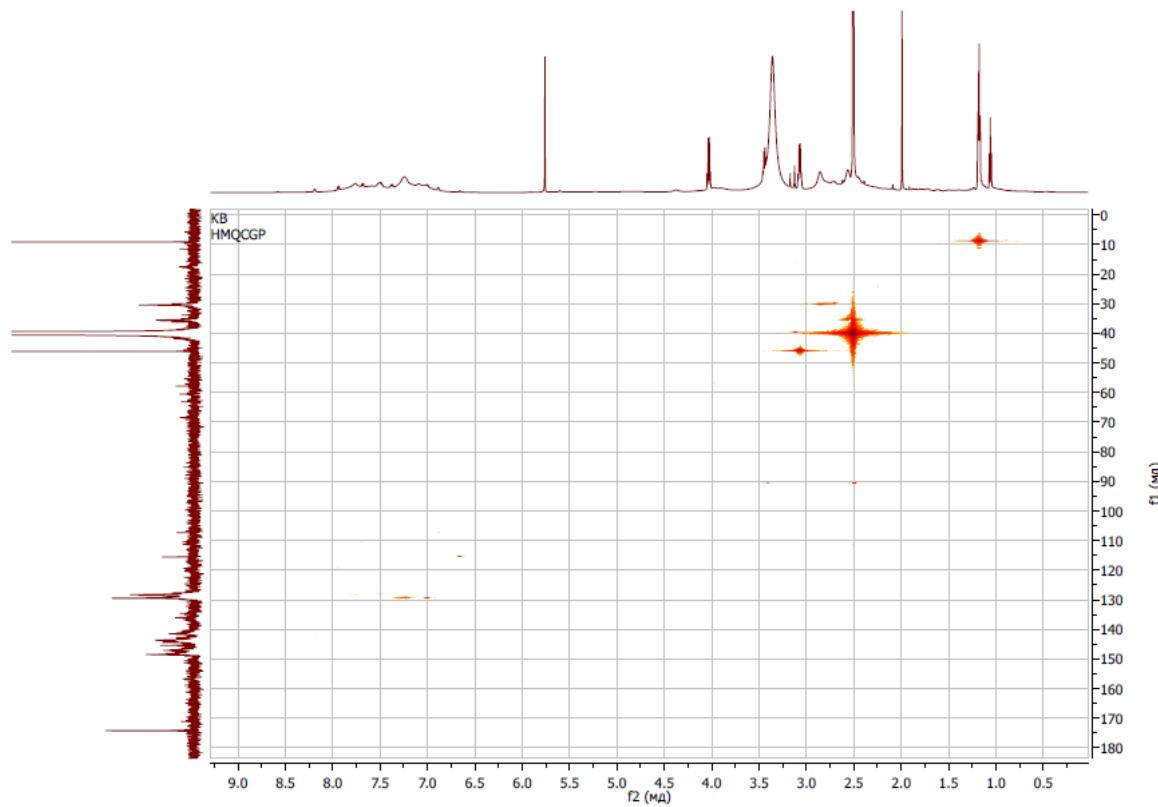
**Fig. S2.** The  $^1\text{H}$  (a) and  $^{13}\text{C}$  NMR (b) spectra of the fullerene-ruboxyl conjugate **4**. Groups of the signals marked with “\*” correspond to the fullerene moiety bearing  $\text{SCH}_2\text{CH}_2\text{COOR}$  groups.



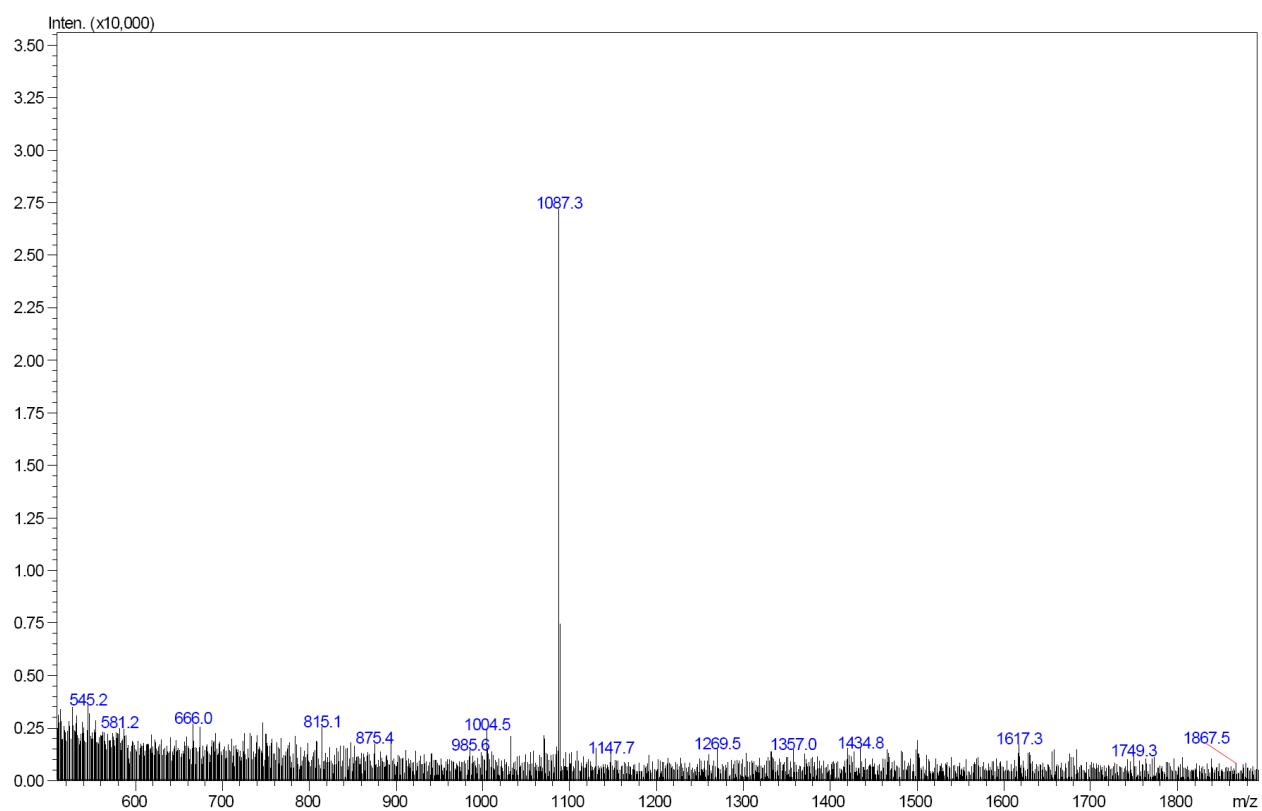
**Fig. S3.** The  $^1\text{H}$  (a) and  $^{13}\text{C}$  NMR (b) spectra of the fullerene-ruboxyl conjugate **5**. Symbol “\*” denotes solvent peaks.



**Fig. S4.** The H-H COSY NMR spectrum of the fullerene-ruboxyl conjugate **5**.



**Fig. S5.** The H-C HMBC NMR spectrum of the fullerene-ruboxyl conjugate **5**.



**Fig. S6.** ESI mass-spectrum of conjugate 5