

## Supporting Information

### Design, synthesis, and biological activity of novel ammonium salts containing sterically hindered phenolic fragment and phosphoryl group

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## Biological evaluation

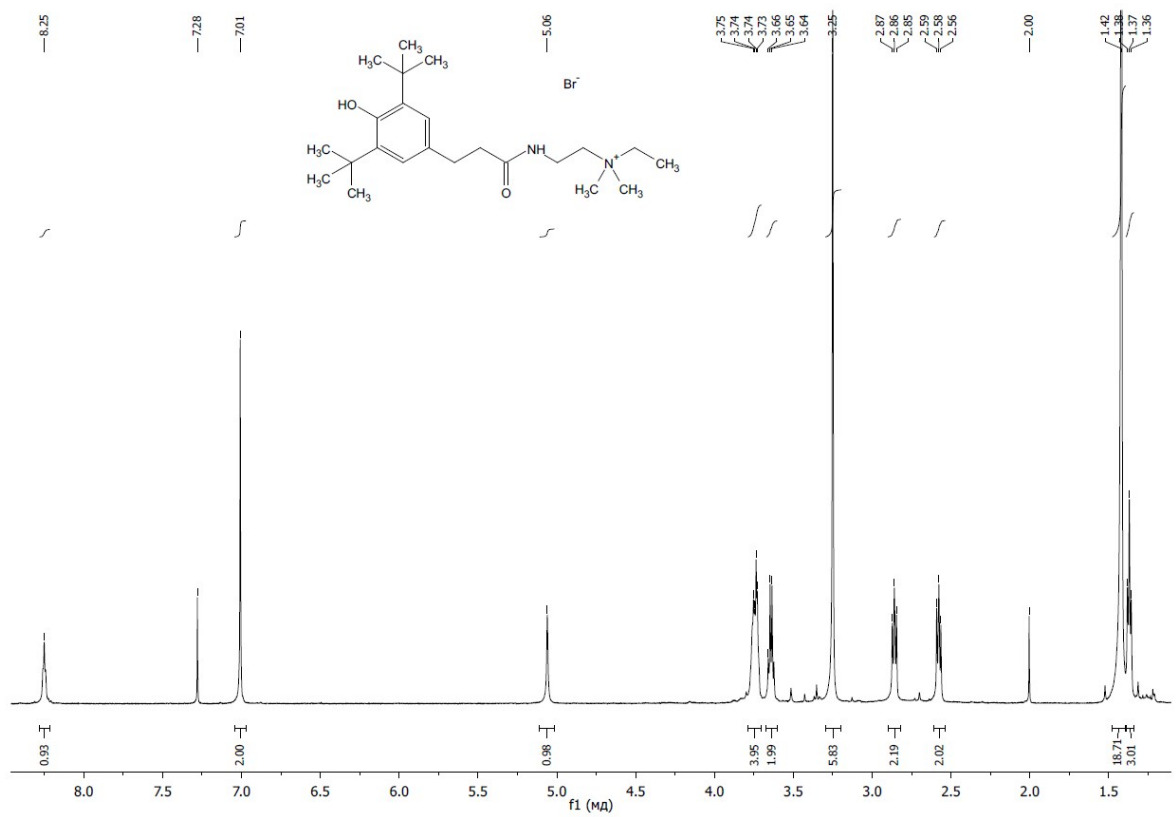
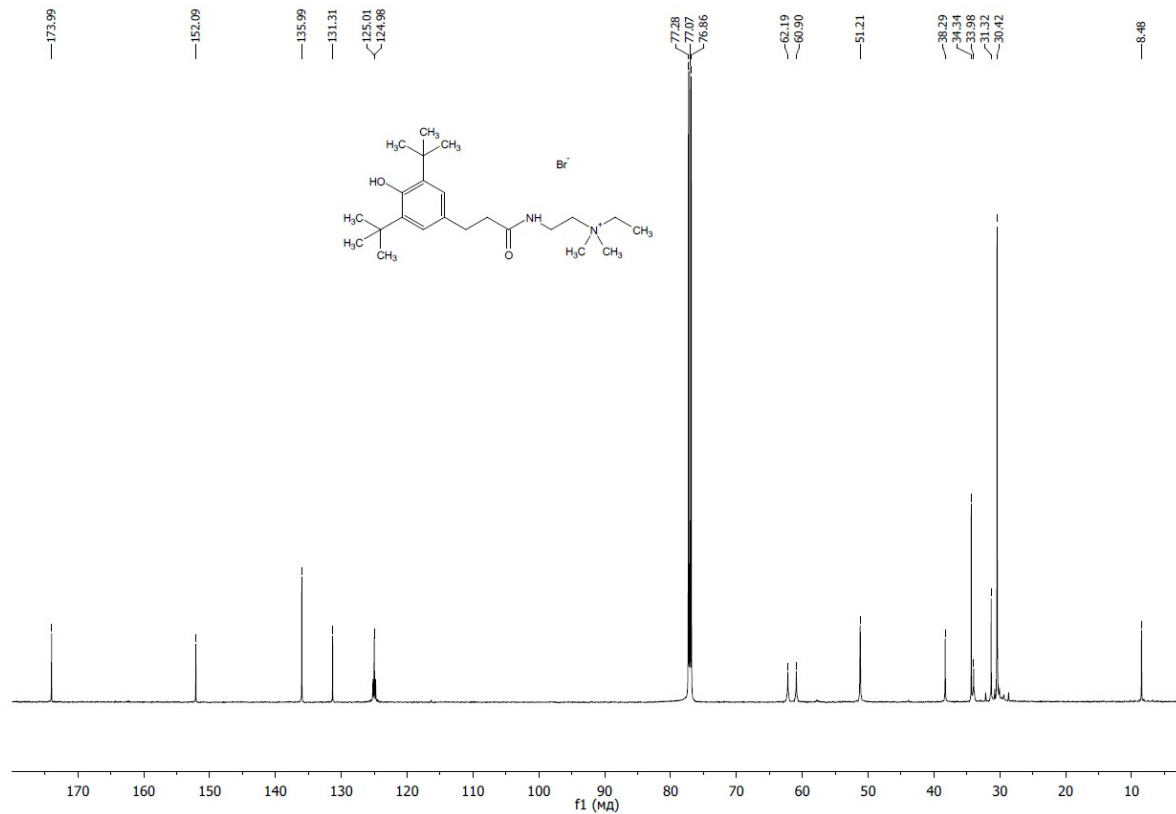
### Antimicrobial activity

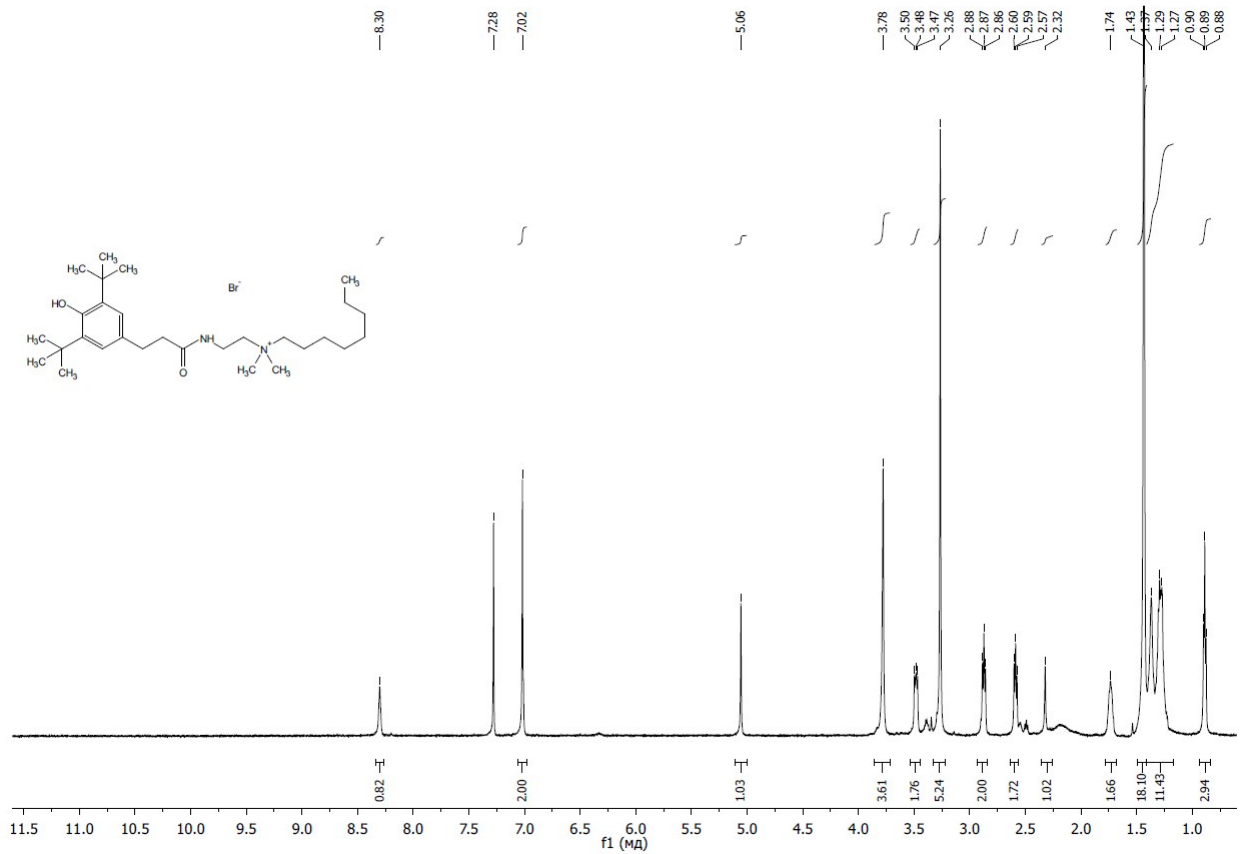
The bacteriostatic activity of the compounds toward *Pseudomonas aeruginosa* ATCC 9027, *Escherichia coli* CDC F-50, *Staphylococcus aureus* ATCC 209p and *Bacillus cereus* ATCC 8035 was determined by the method of twofold serial dilutions in a liquid nutrient medium. The bacterial load was  $3.0 \times 10^5$  microbial bodies mL<sup>-1</sup>. The results were recorded every 24 h for 5 days. Cultures were incubated at 37°C. The experiment was repeated twice. The fungistatic activity of aqueous solutions of the compounds toward the fungi *Trichophyton mentagrophytes* var. *gypseum* 1773, *Aspergillus niger* BKMF-1119 and *Candida albicans* 855-653A was determined by the method of serial dilutions on Sabouraud liquid medium. The time of the exposure in a thermostat at 25°C with the corresponding compound was 14 days. The dilutions of the compounds were prepared immediately in nutrient media; for better solubility, 5% DMSO was added, which does not induce the inhibition of test strains at this concentration. The MIC was defined as the minimal concentration of a compound that inhibits the growth of the corresponding test microorganism. The growth of bacteria and fungi as well as the absence of the growth owing to the bacteriostatic and fungistatic action of a compound were recorded. The bactericidal and fungicidal activities were determined as described earlier.

### Cytotoxicity

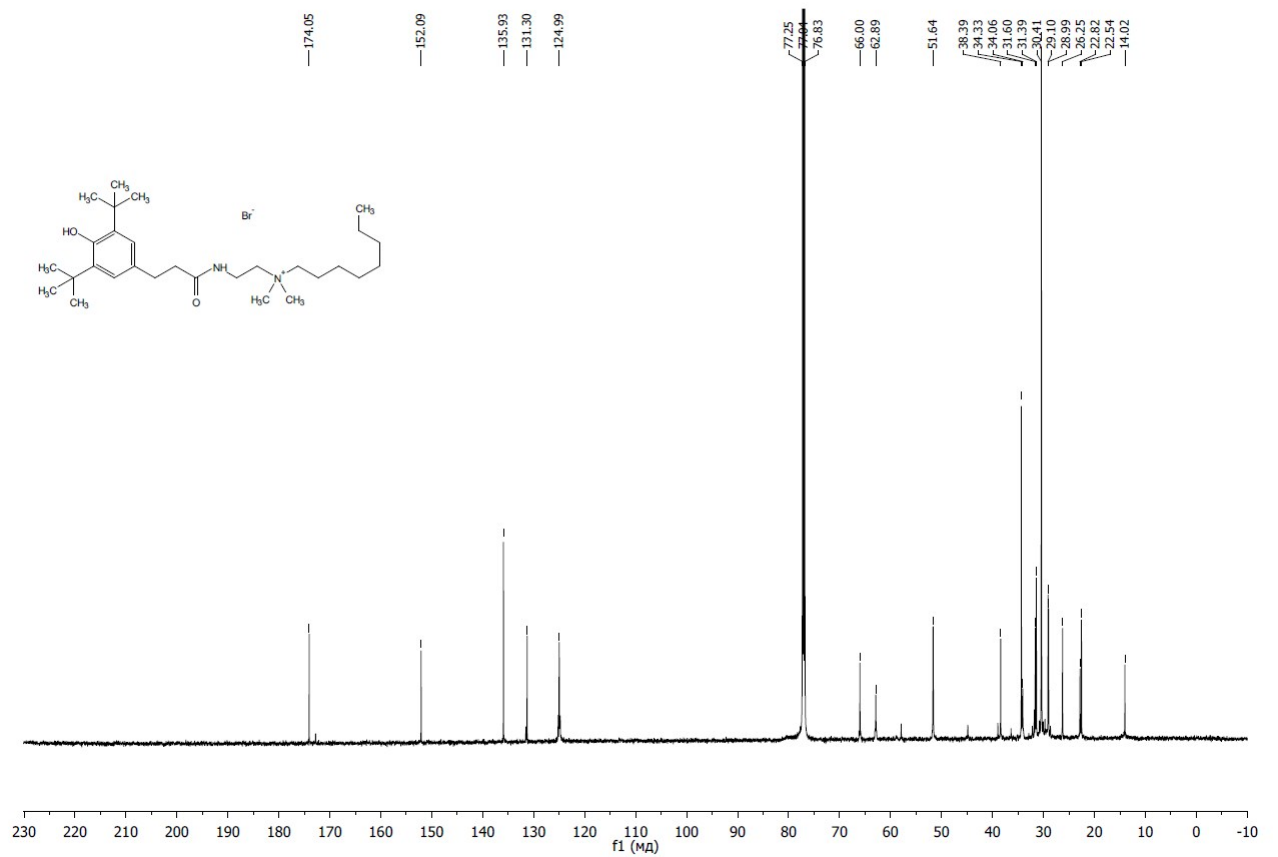
The cytotoxicity of the compounds at the MIC, which inhibits the growth of bacterial and fungal test strains, was estimated by counting the viable WI-38 and Chang liver cells, as compared with the control, by the Cytell Cell Imaging multifunctional system (GE Health Care Life Science, Sweden) using the Cell Viability BioApp application, which makes it possible to precisely count the number of cells and estimate their viability from the fluorescence intensity with the use of disposable hemocytometer. The WI-38 VA 13 cell culture, subline 2RA (human embryonic lung) and Chang liver (human liver cells), from the Collection of the Institute of Cytology (Russian Academy of Sciences) was used for experiments. Cells were cultured in a standard Eagle's nutrient medium manufactured at the Chumakov Institute of Poliomyelitis and Virus Encephalitis (PanEco company) and supplemented with 10% fetal calf serum and 1% nonessential amino acids. WI-38 cells were plated into a 24-well plate (Eppendorf) at a concentration of 200000 cells/mL, 500  $\mu$ L of medium per well, and cultured in a CO<sub>2</sub> incubator at 37°C. Twenty four hours after seeding the cells into wells, a compound examined was added at a preset dilution, 500  $\mu$ L to each well. The dilutions of the compounds were prepared immediately in nutrient media; for better solubility, 5% DMSO was added, which does not induce the inhibition of WI-38 cells at this concentration. The experiments were performed in triplicates. Intact cells cultured in parallel with experimental cells served as a control.

**<sup>1</sup>H, <sup>13</sup>C NMR spectra compounds of 4a–e, 5a–e**

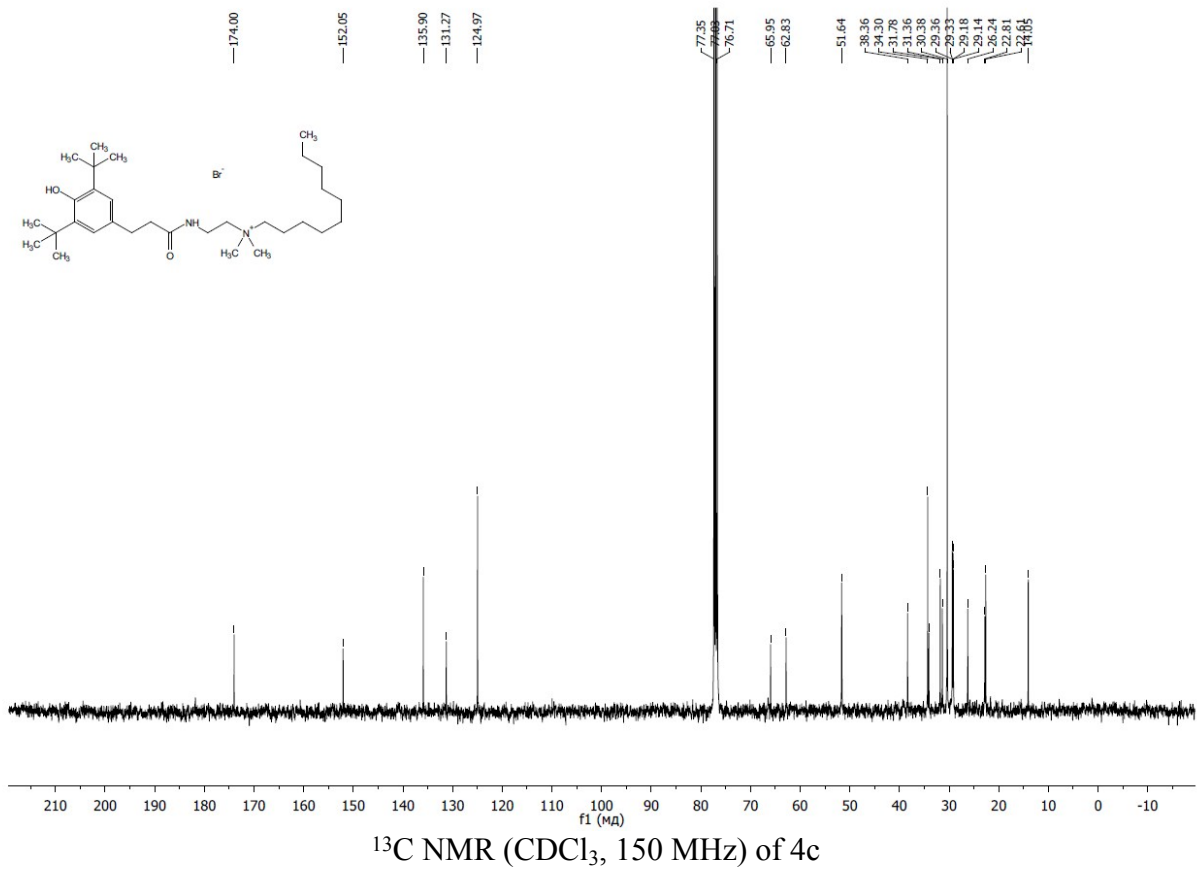
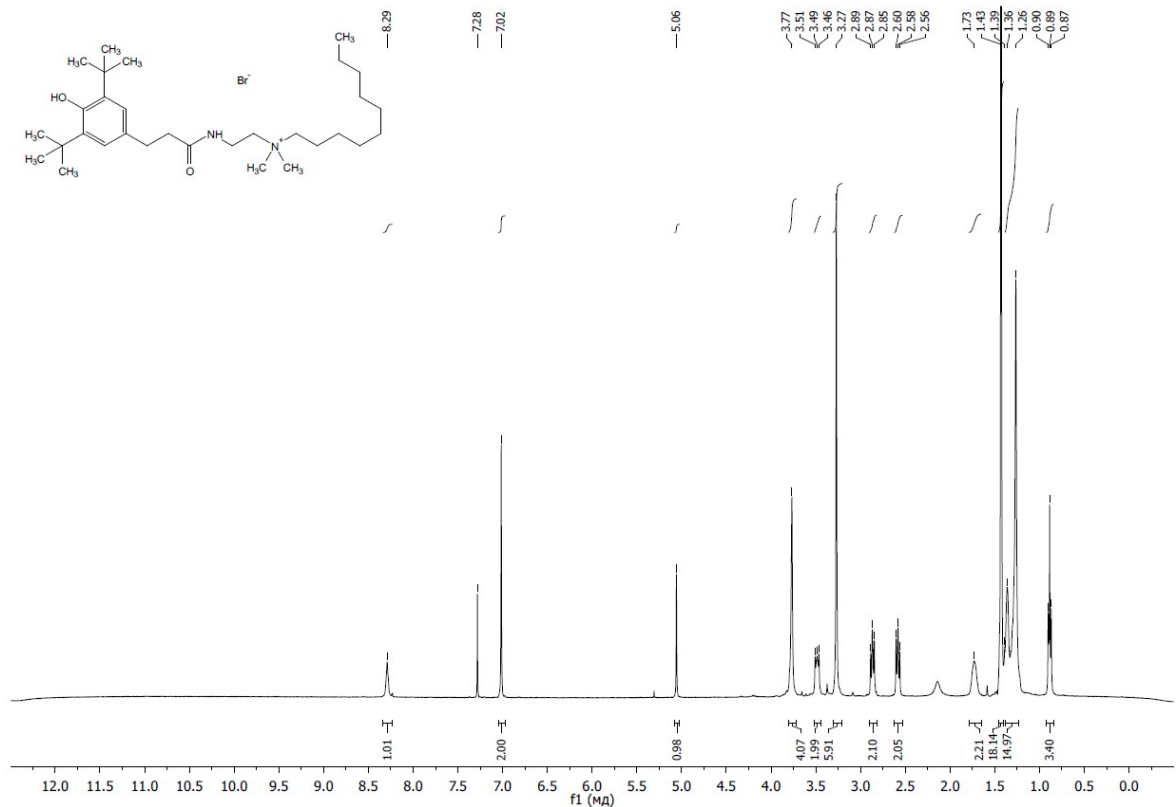
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400.13 MHz) of 4a<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz) of 4a

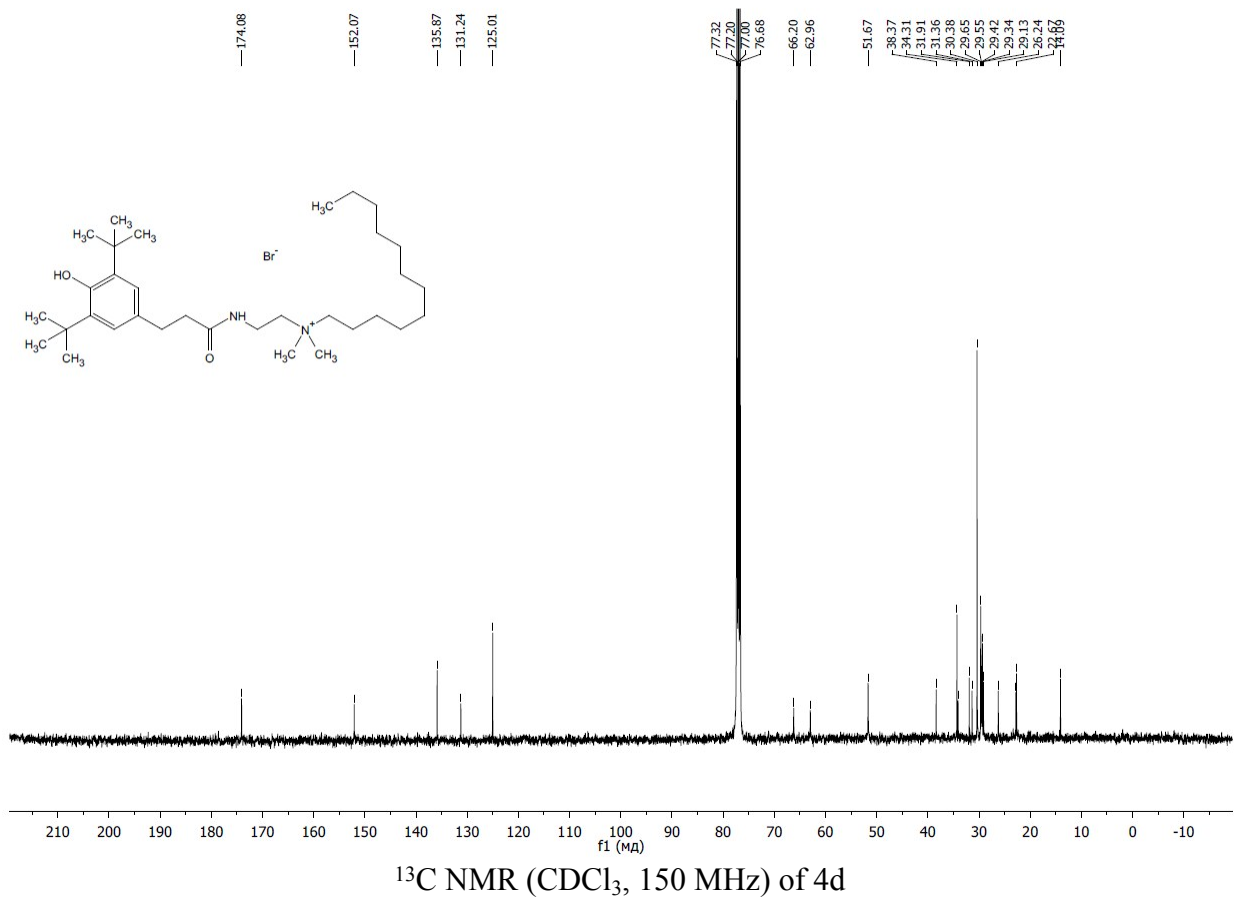
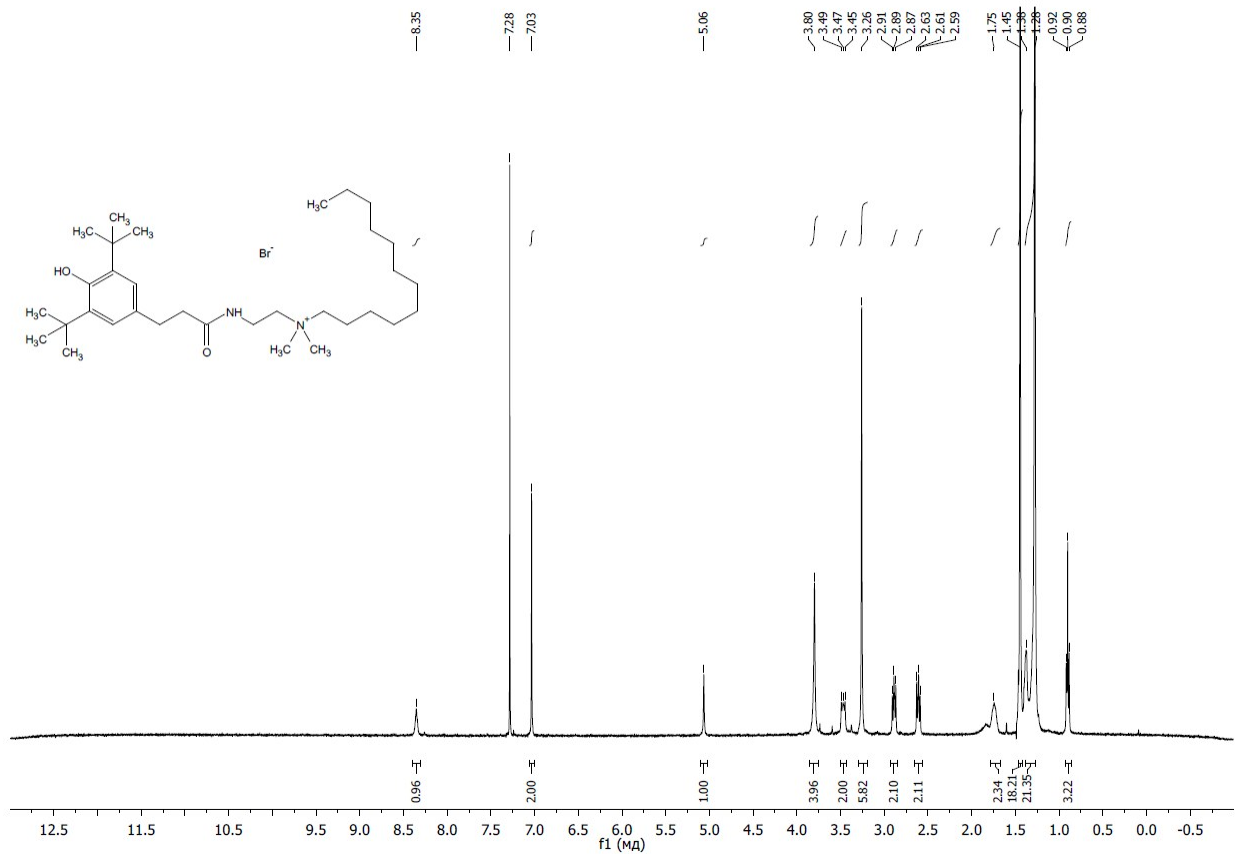


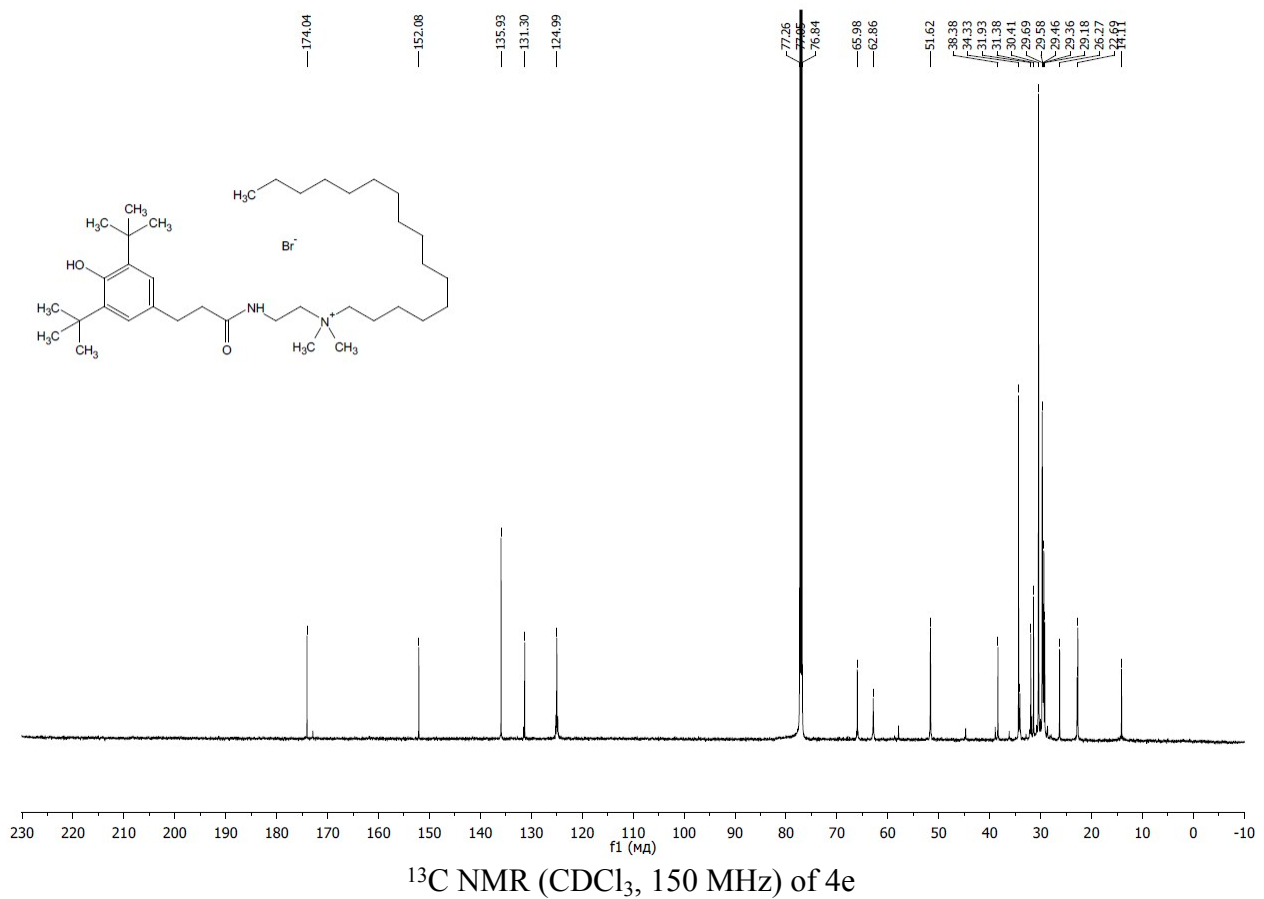
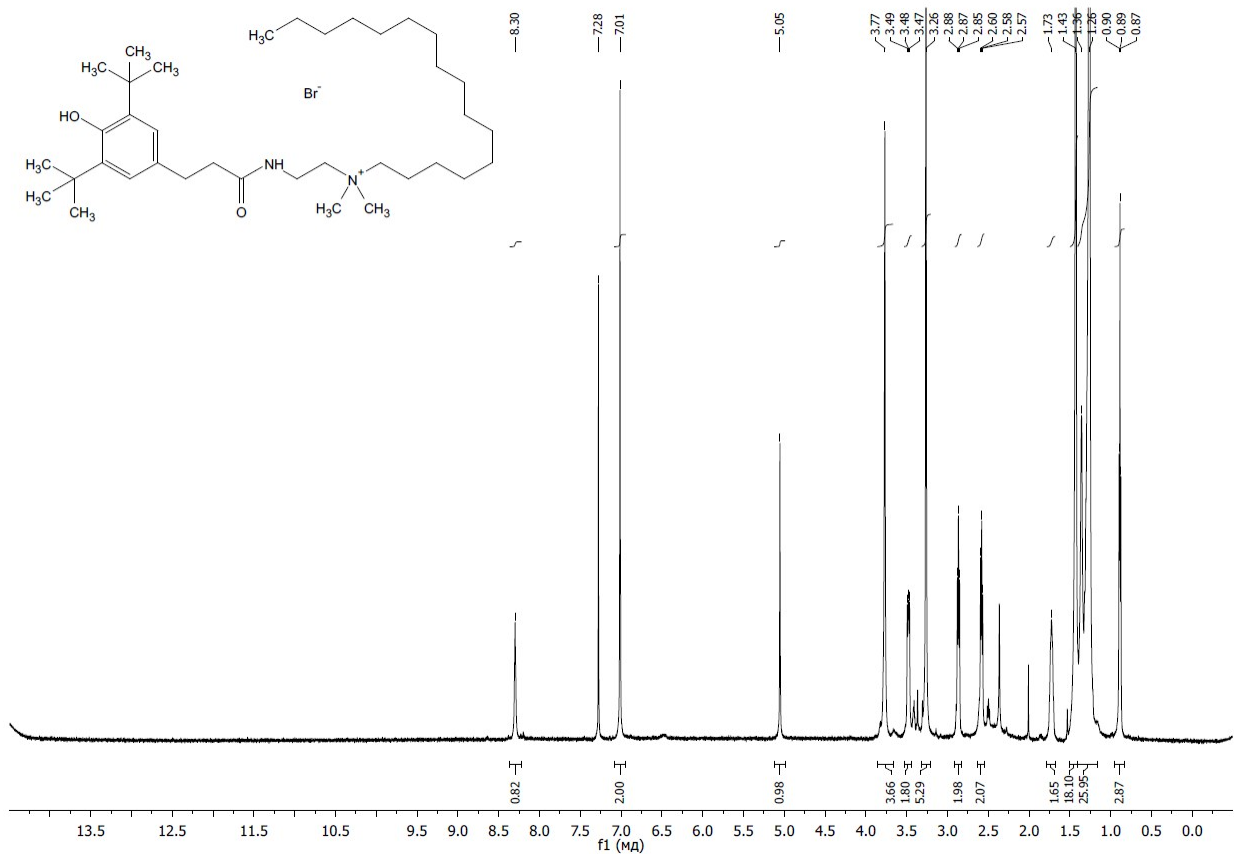
**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400.13 MHz) of 4b**

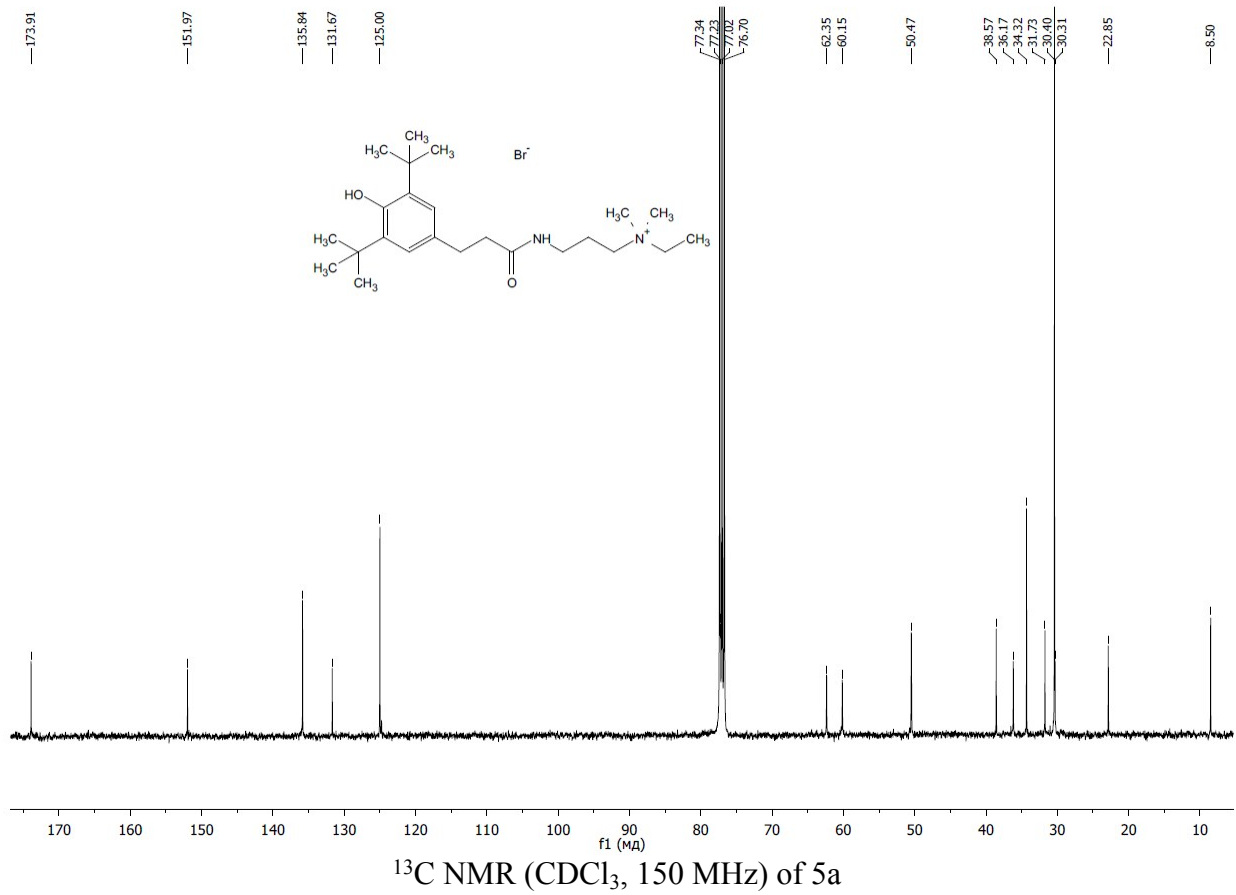
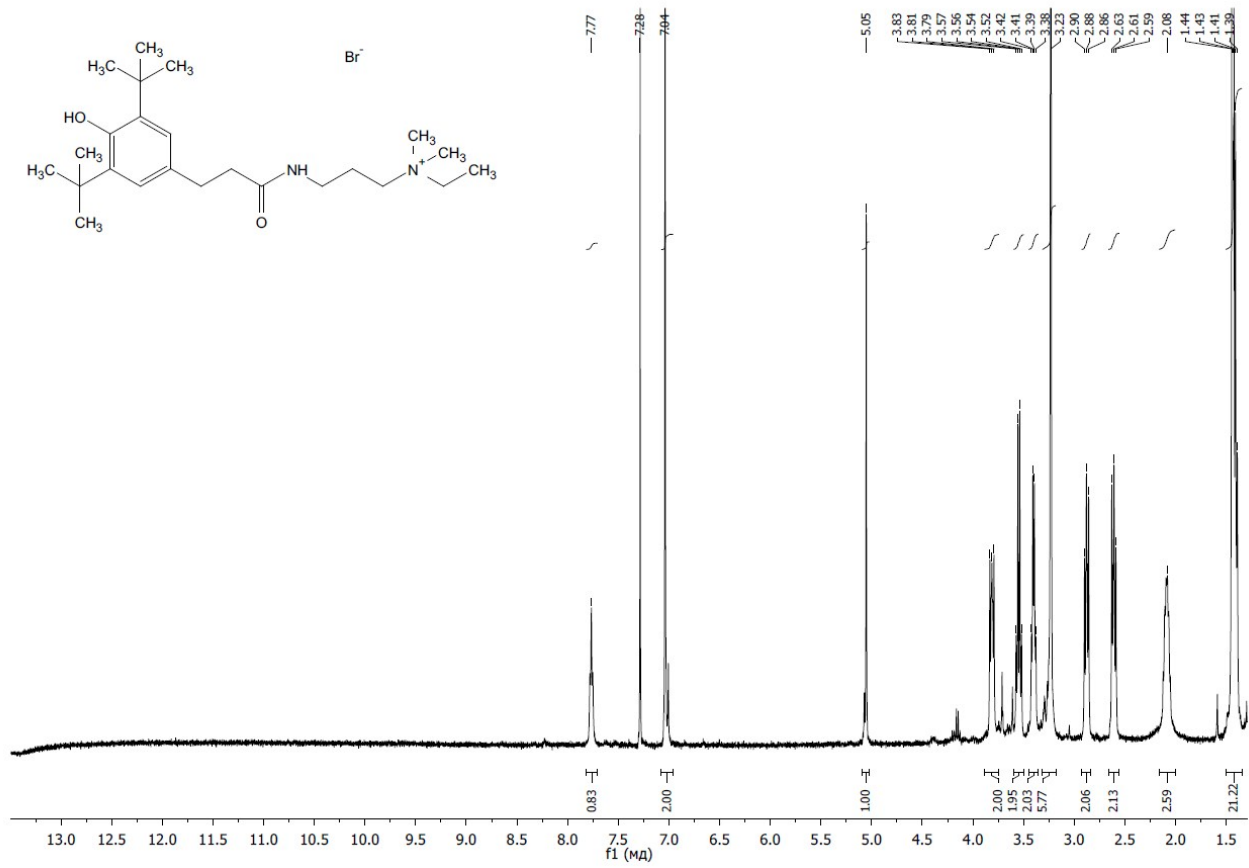


**<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz) of 4b**

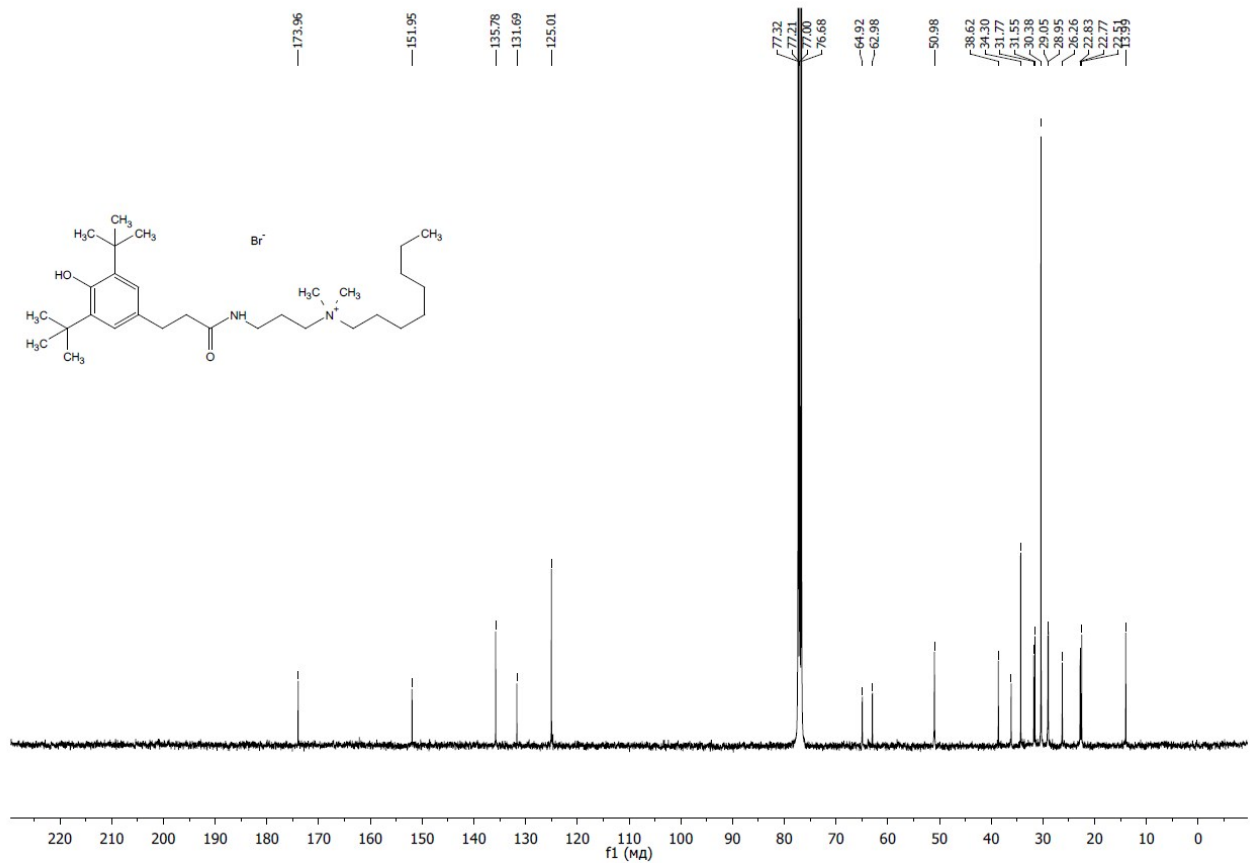
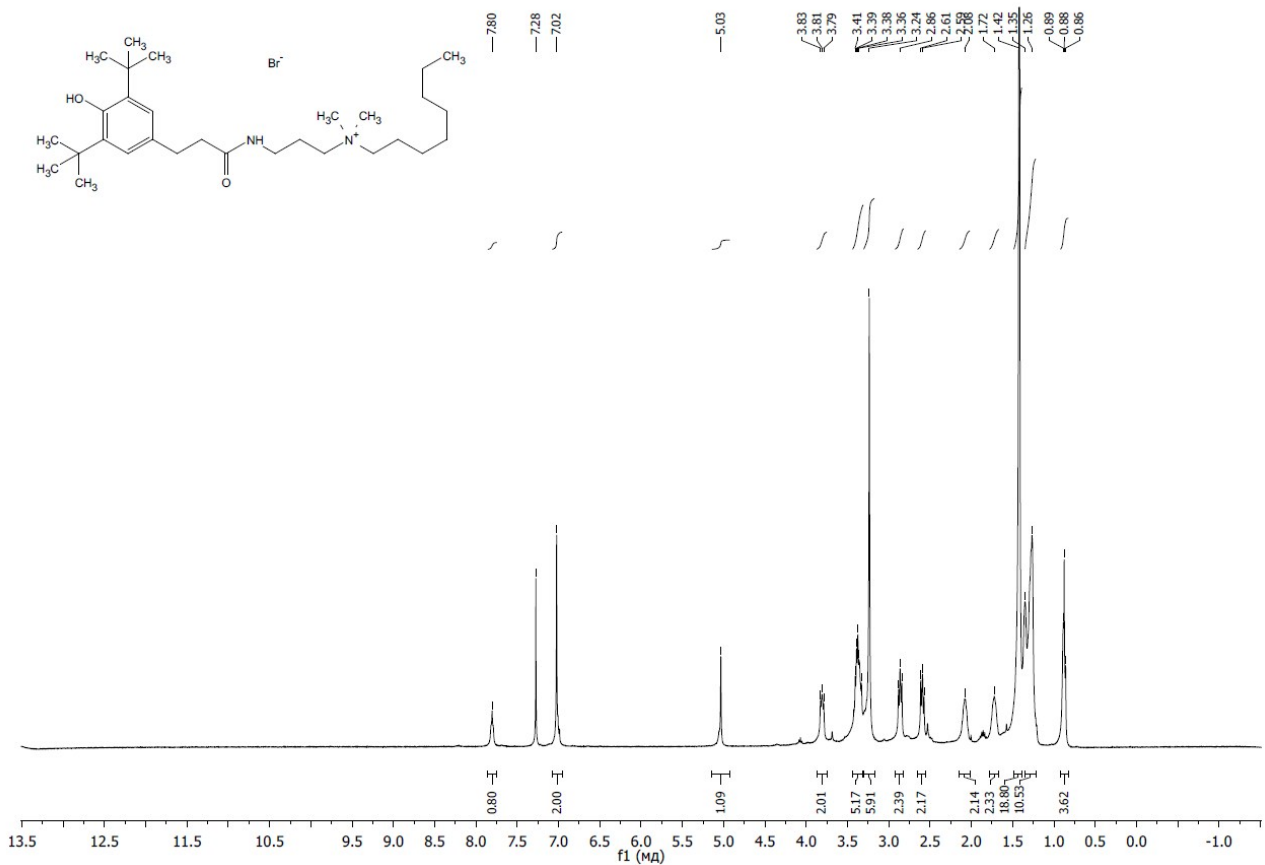


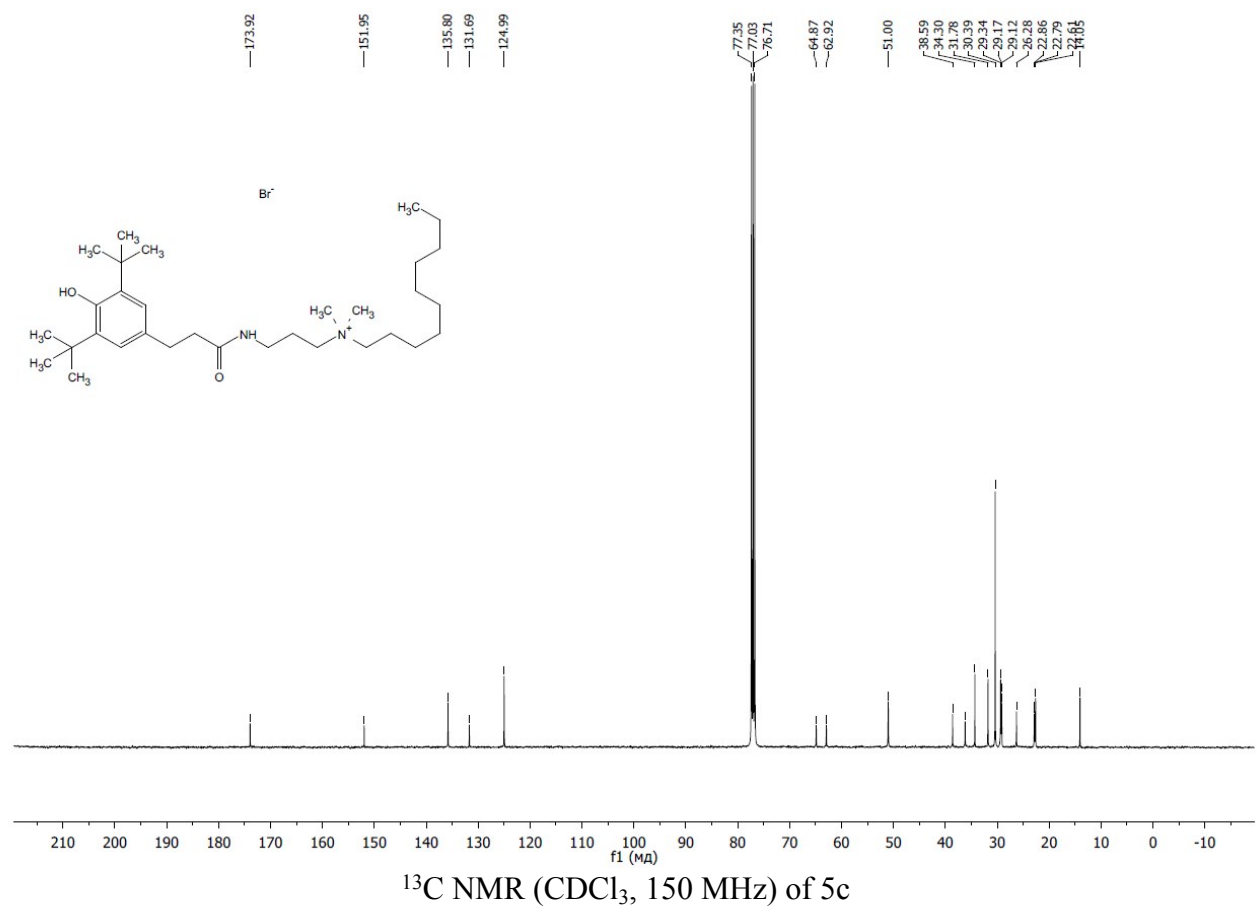
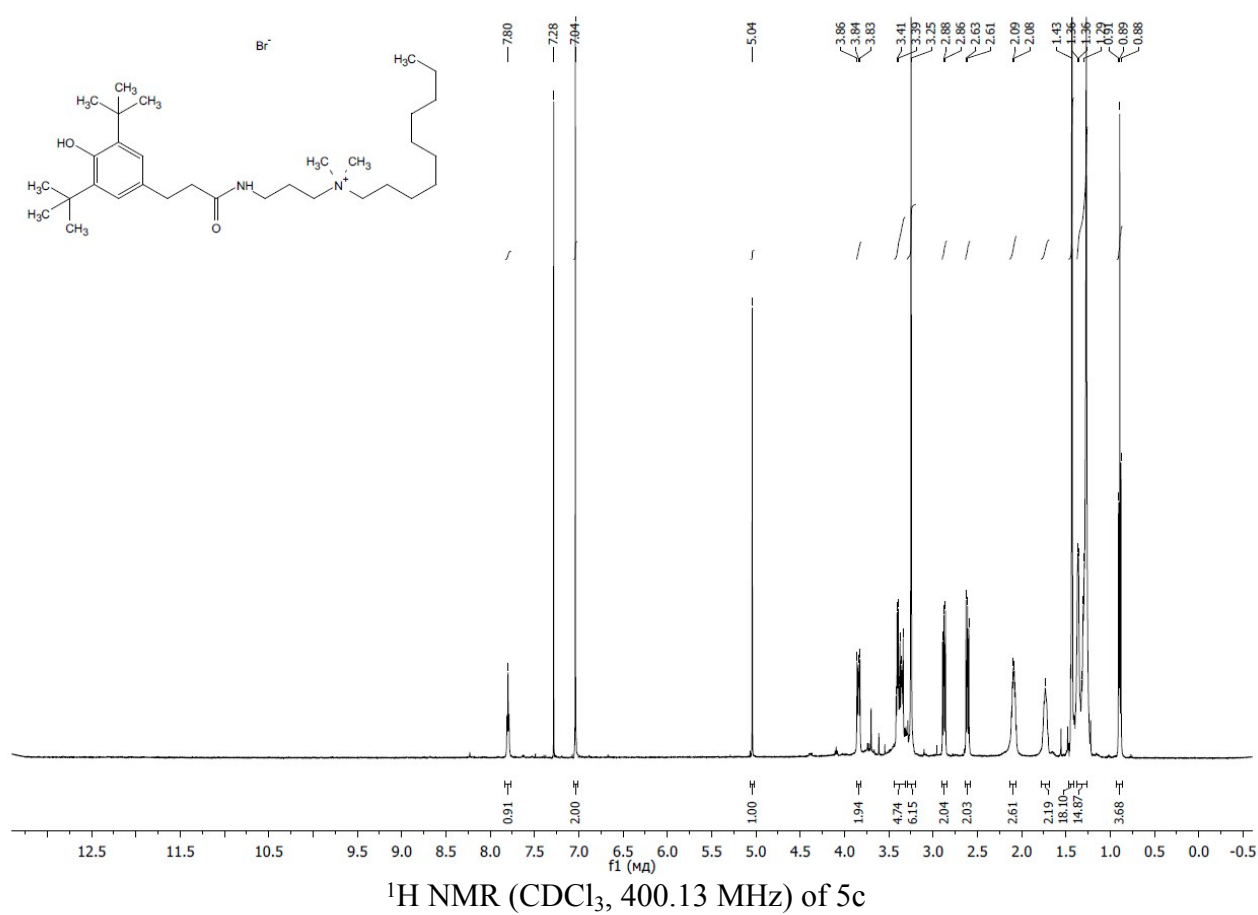


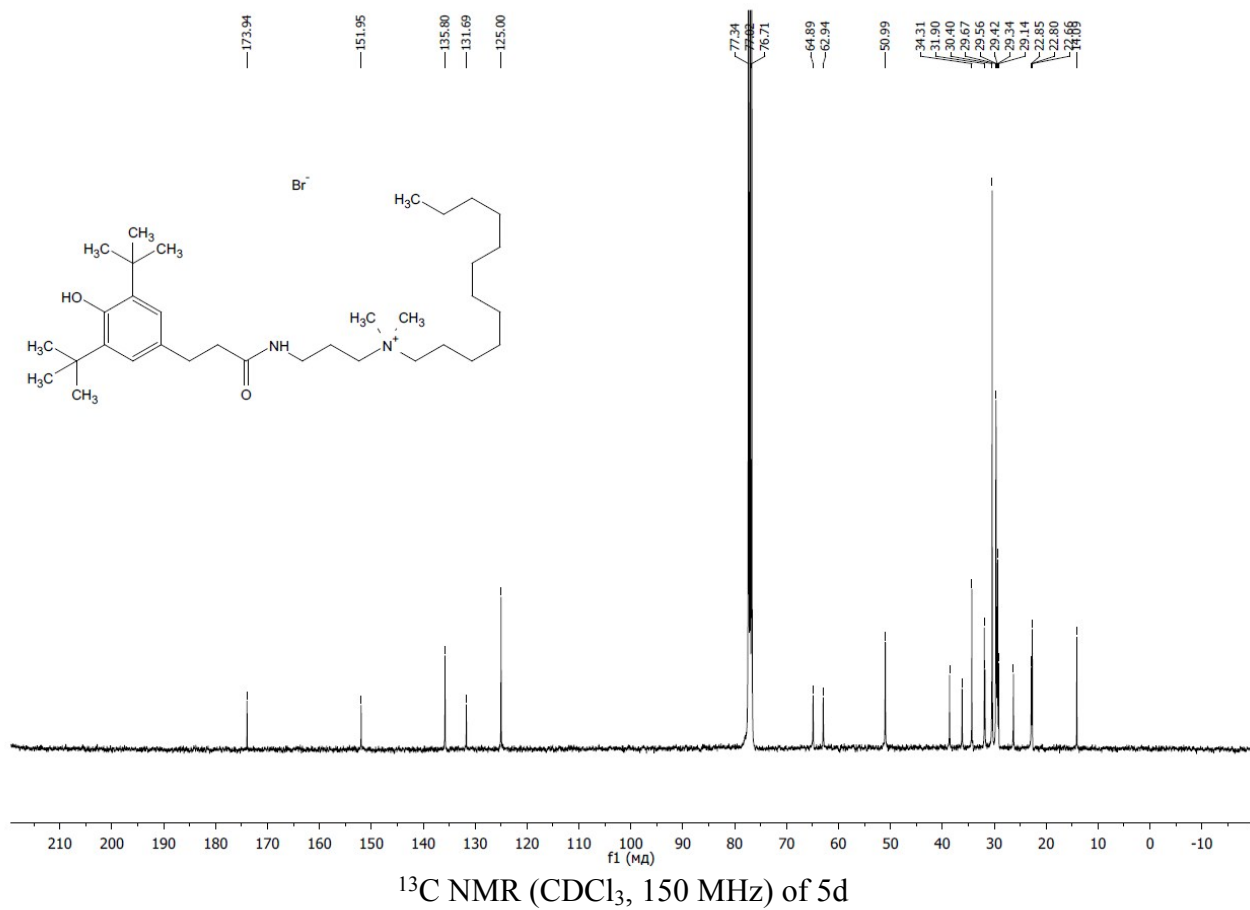
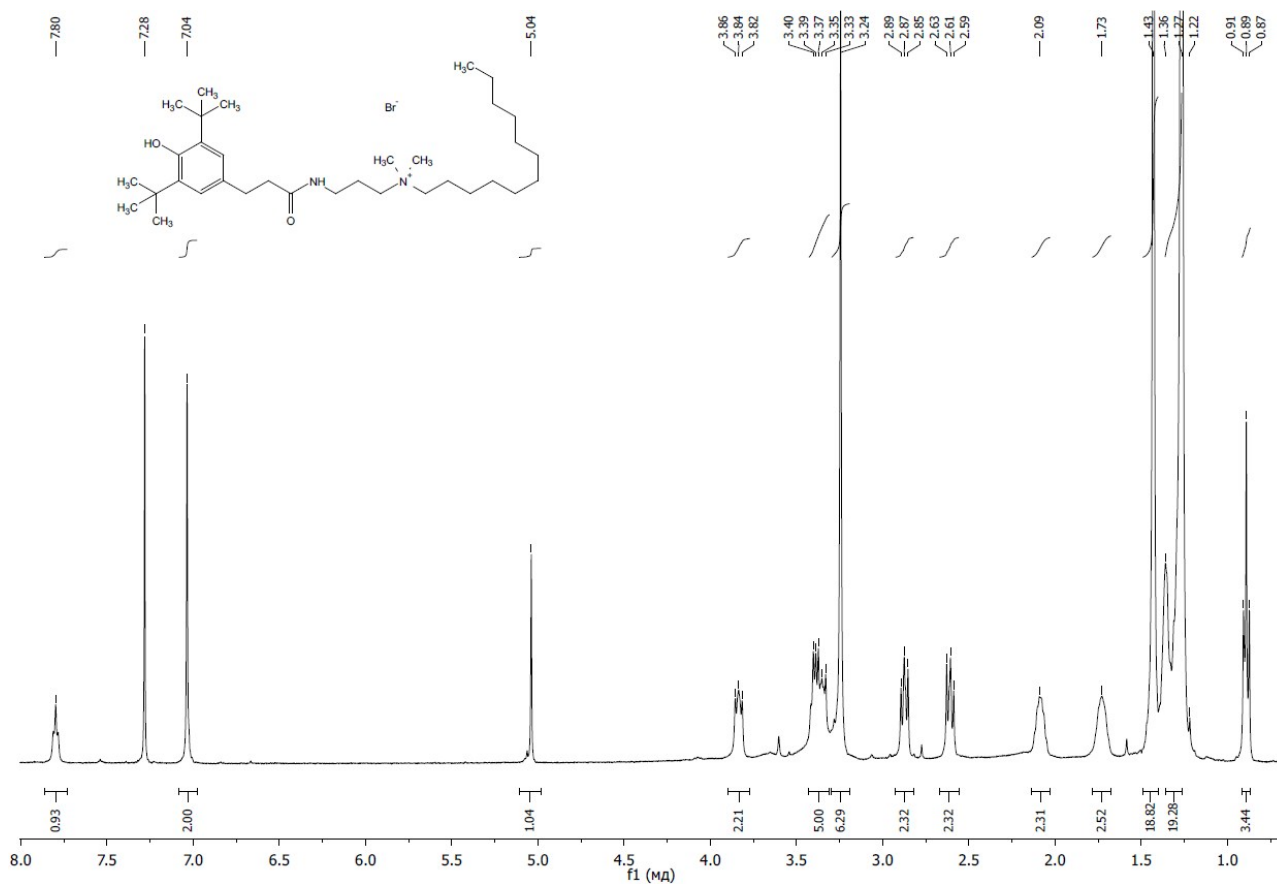


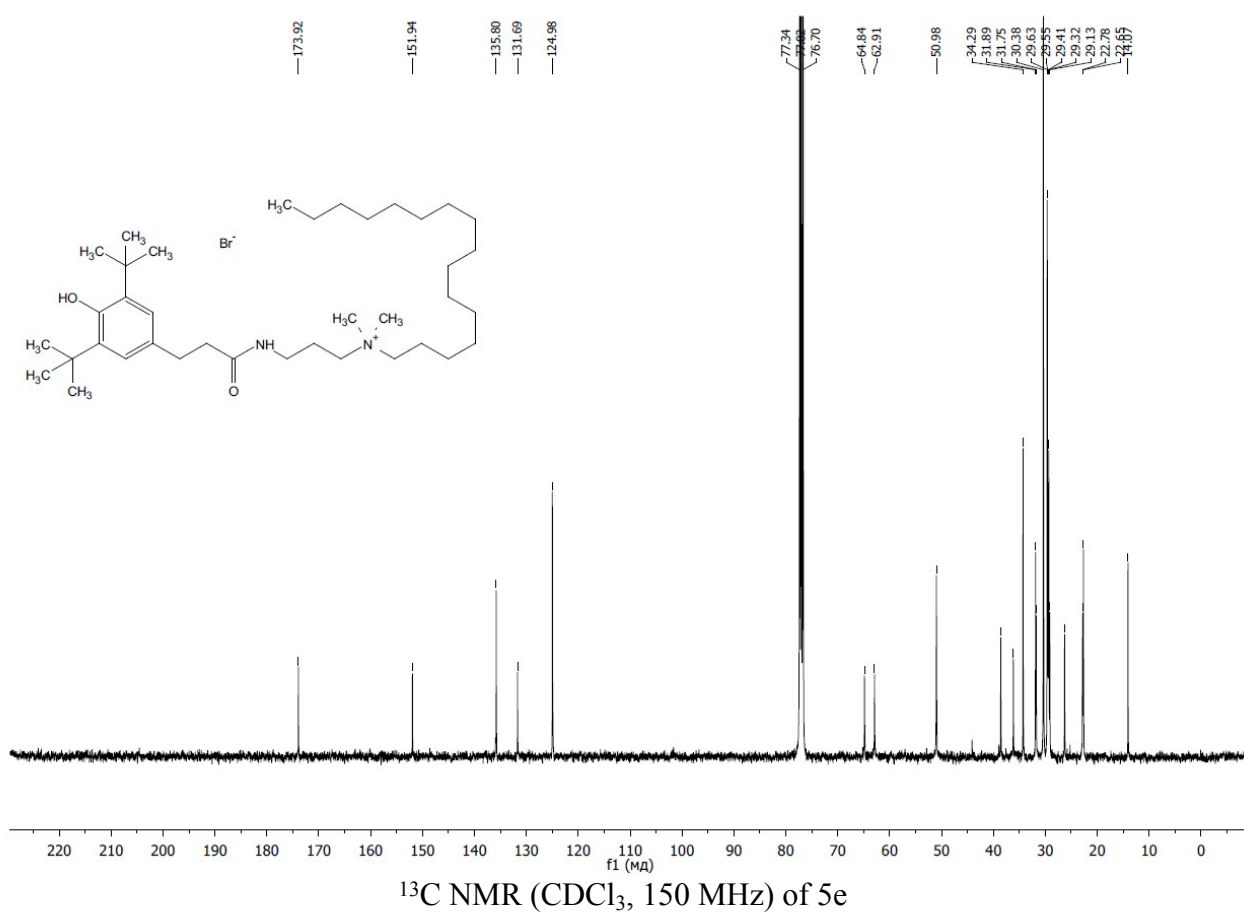
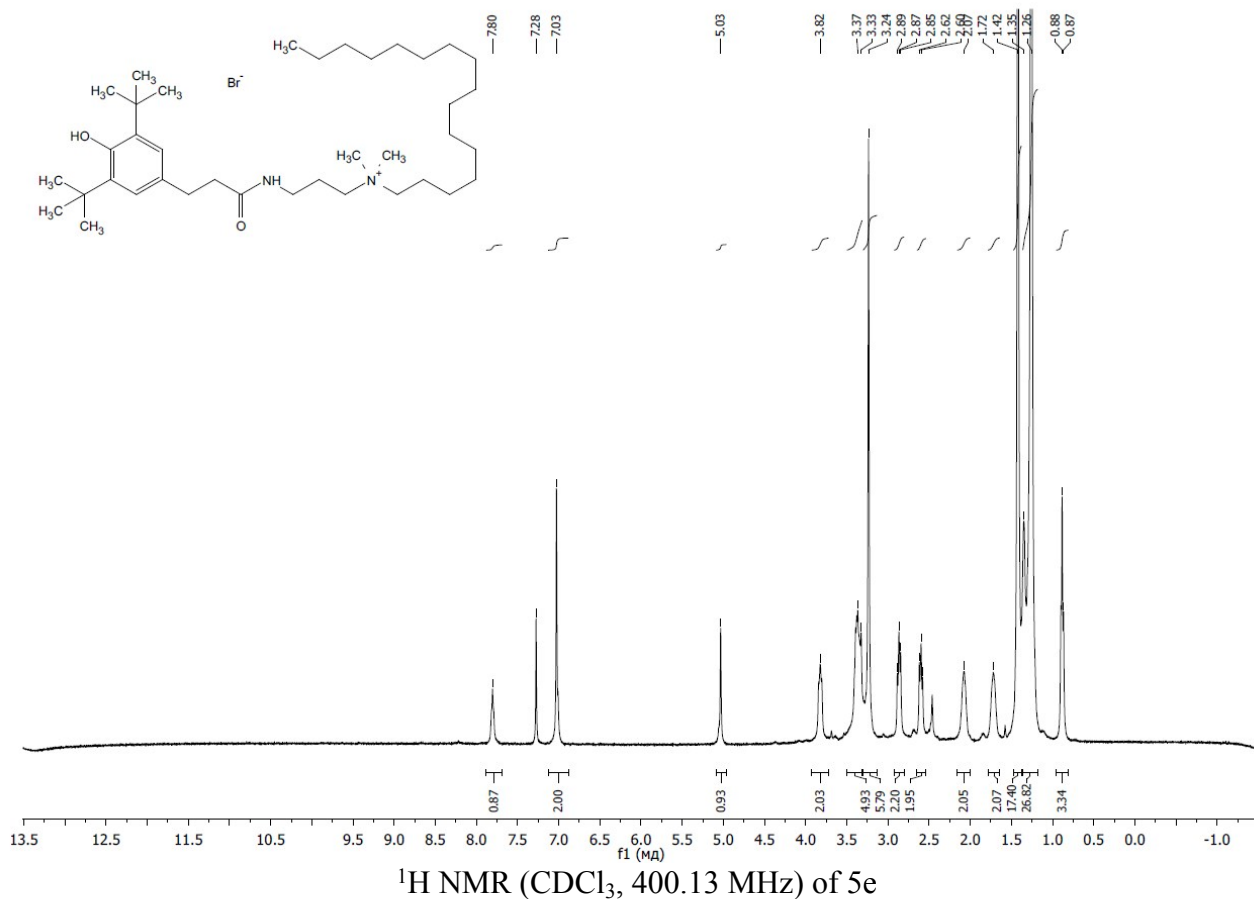


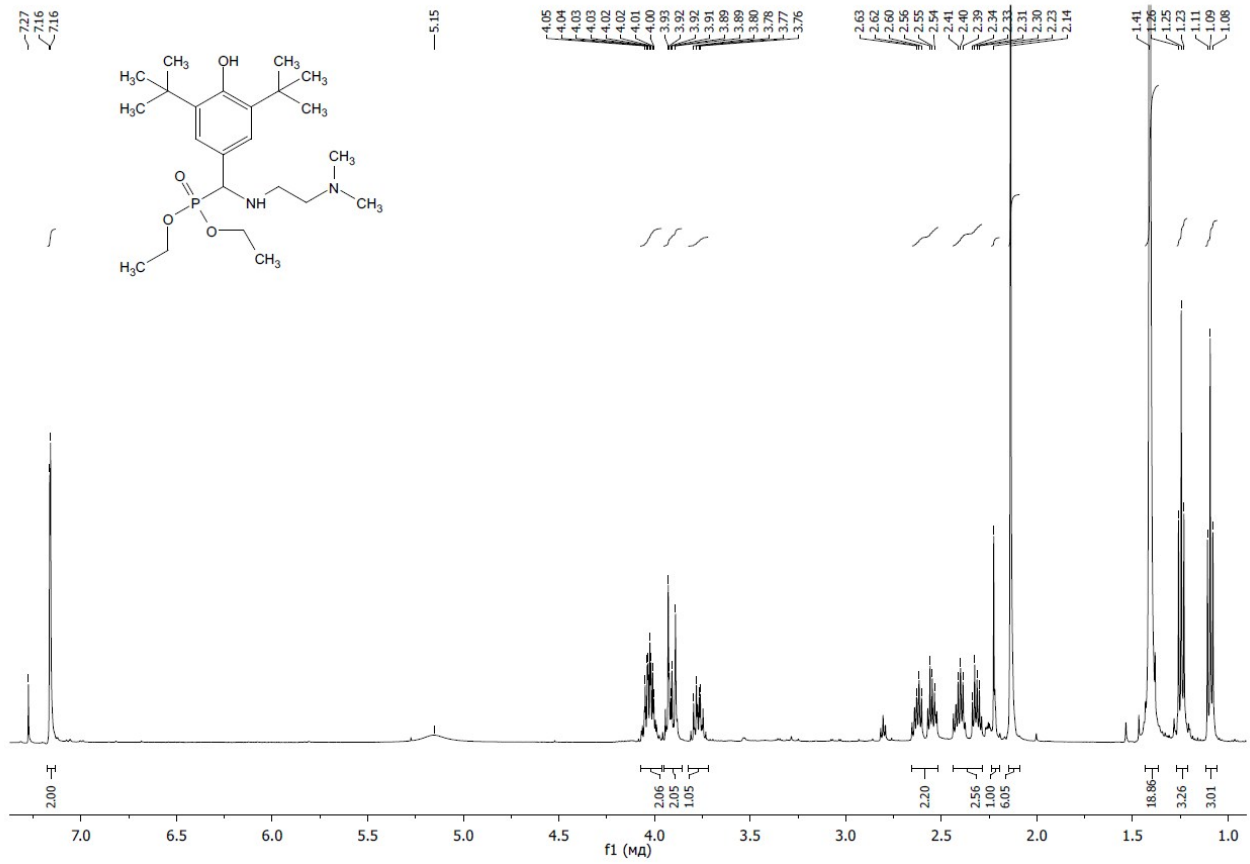


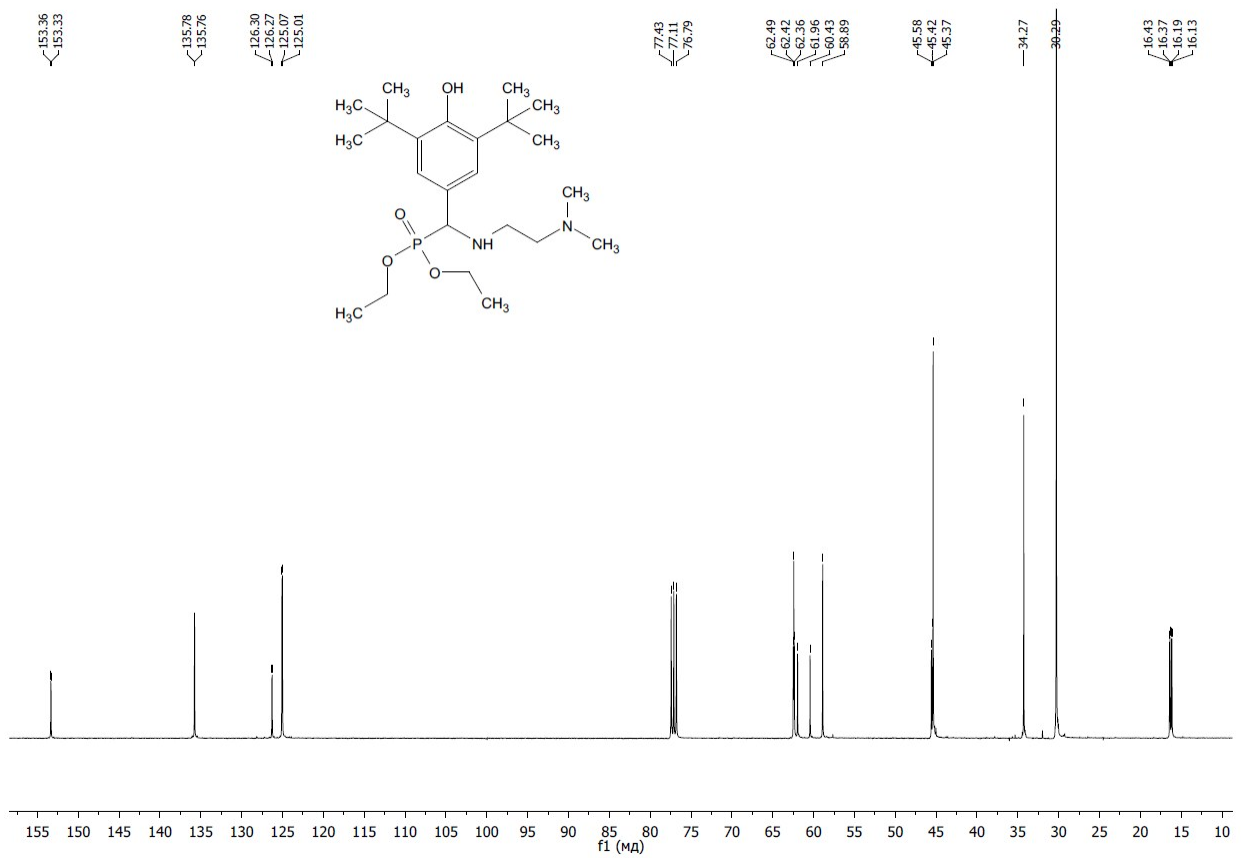




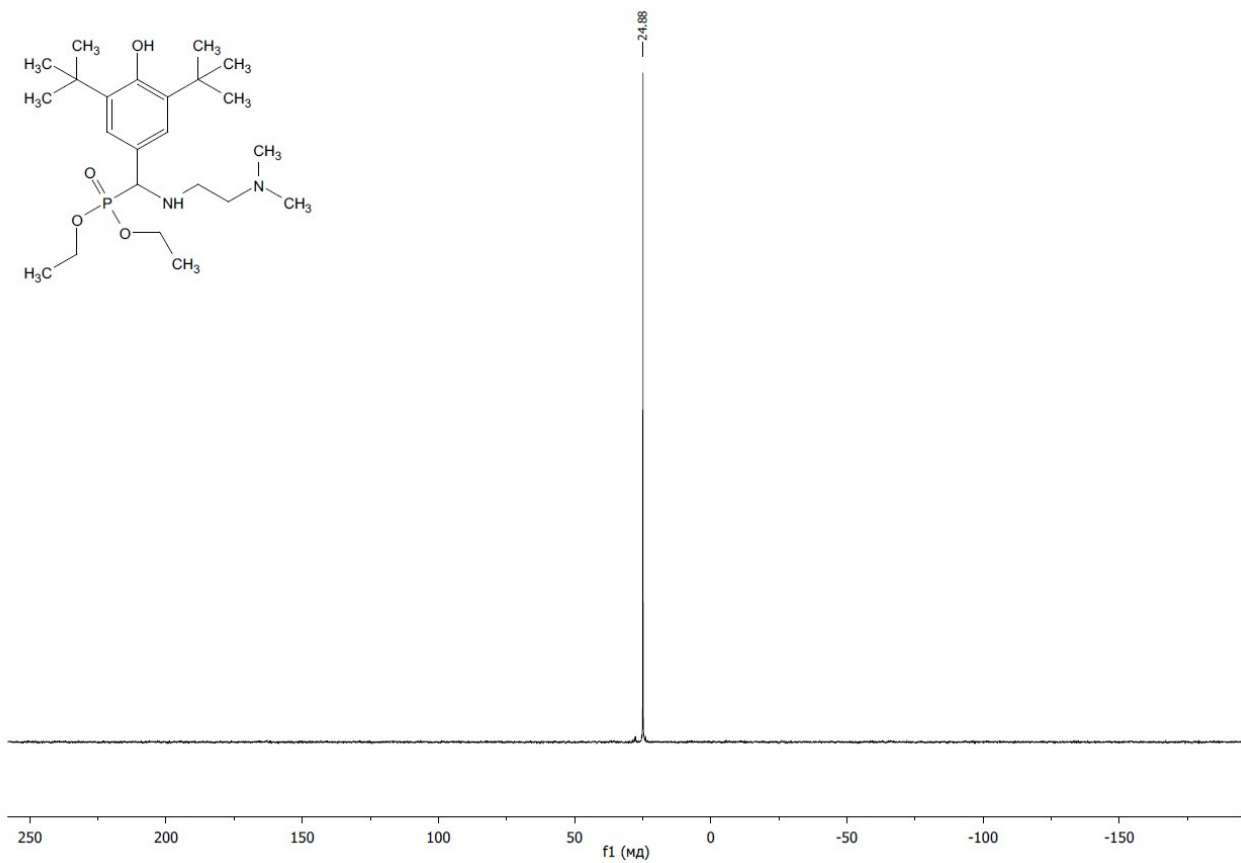


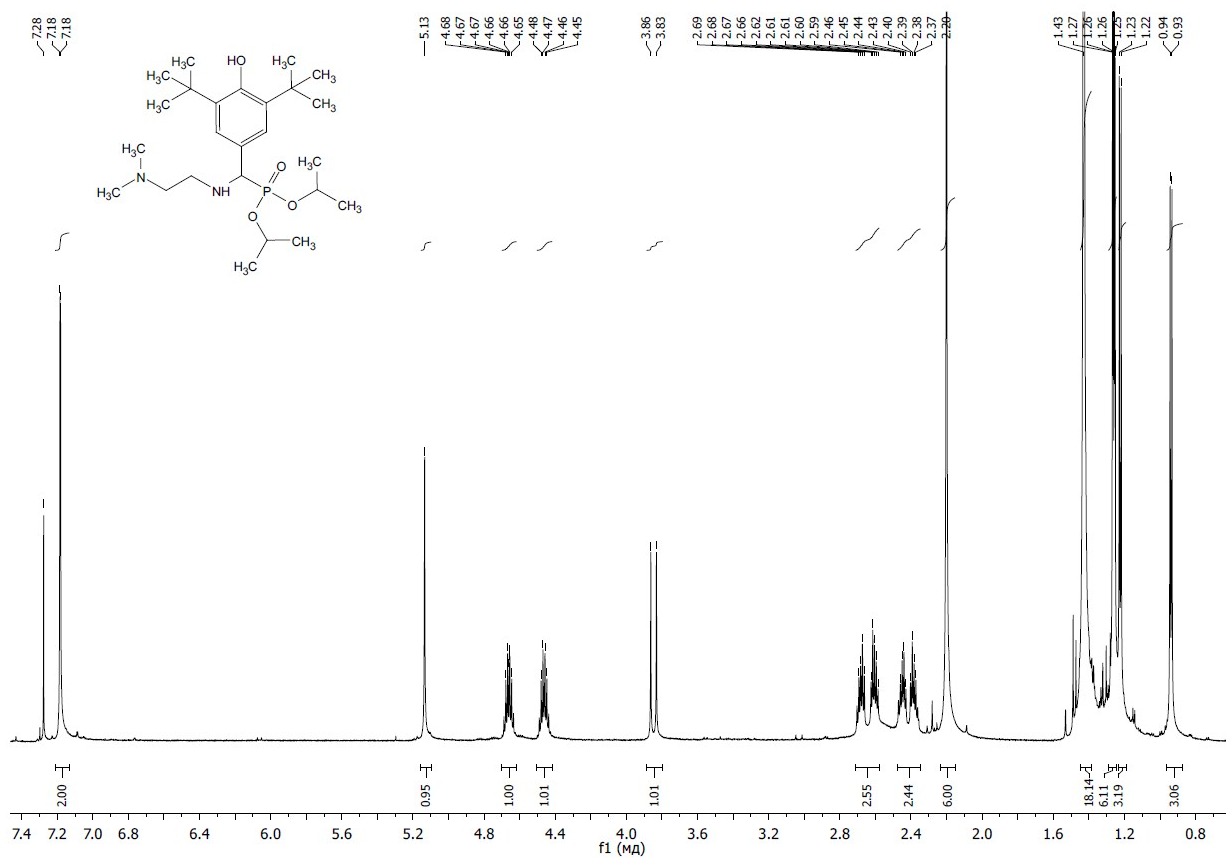
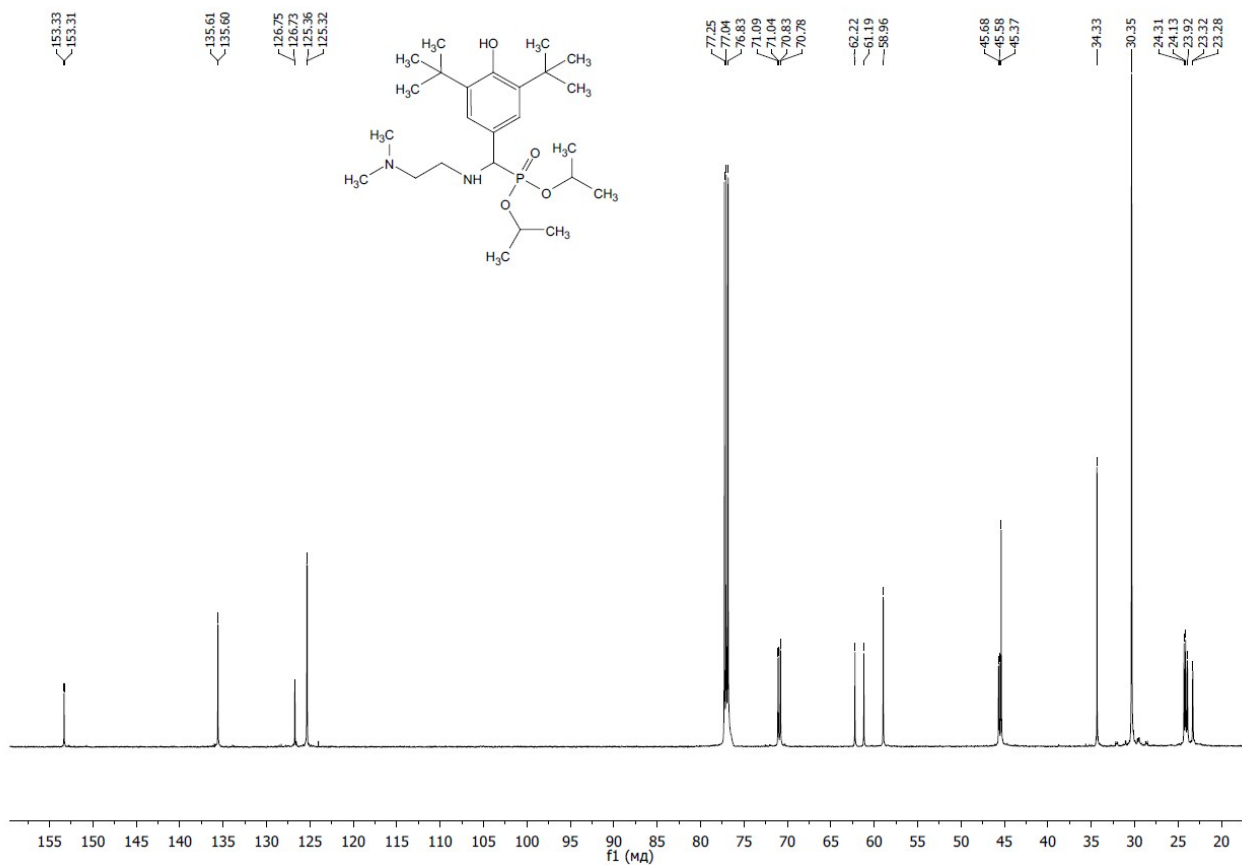


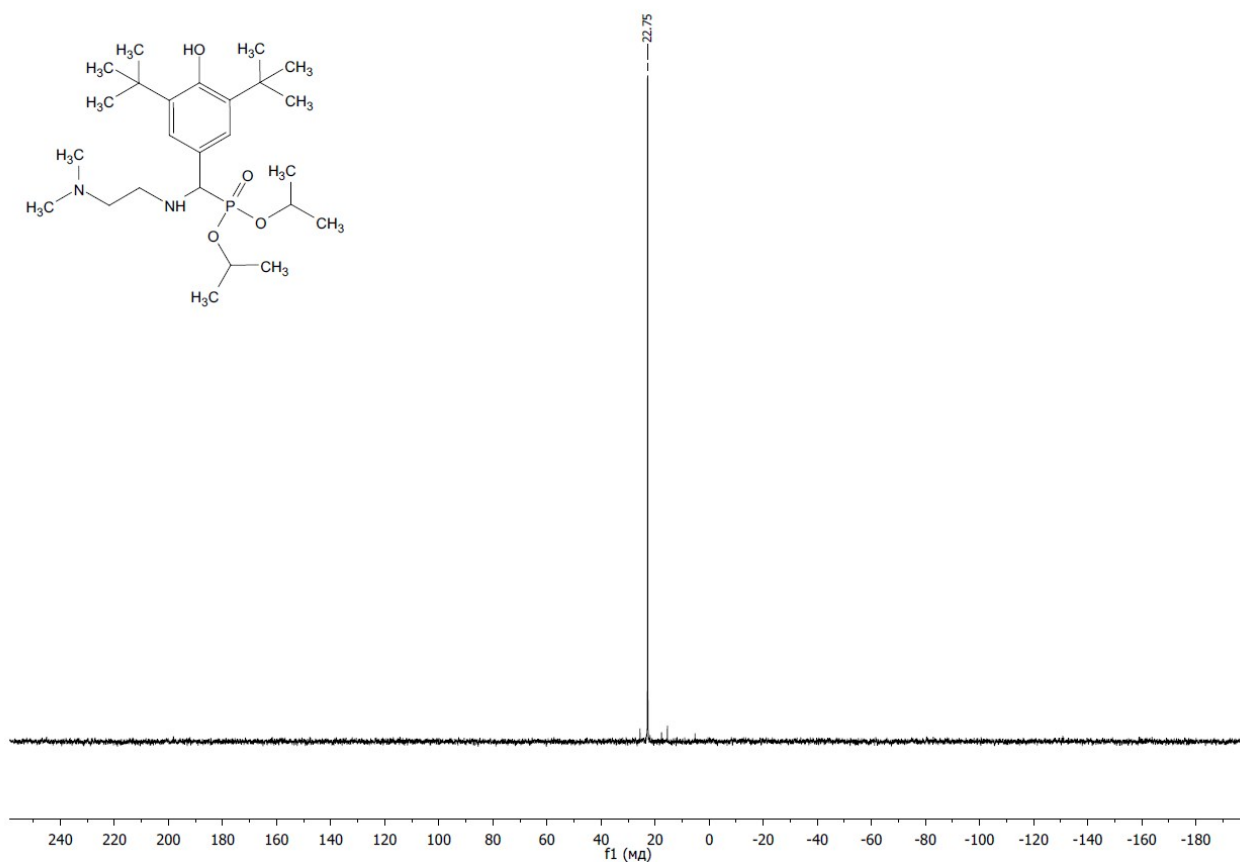
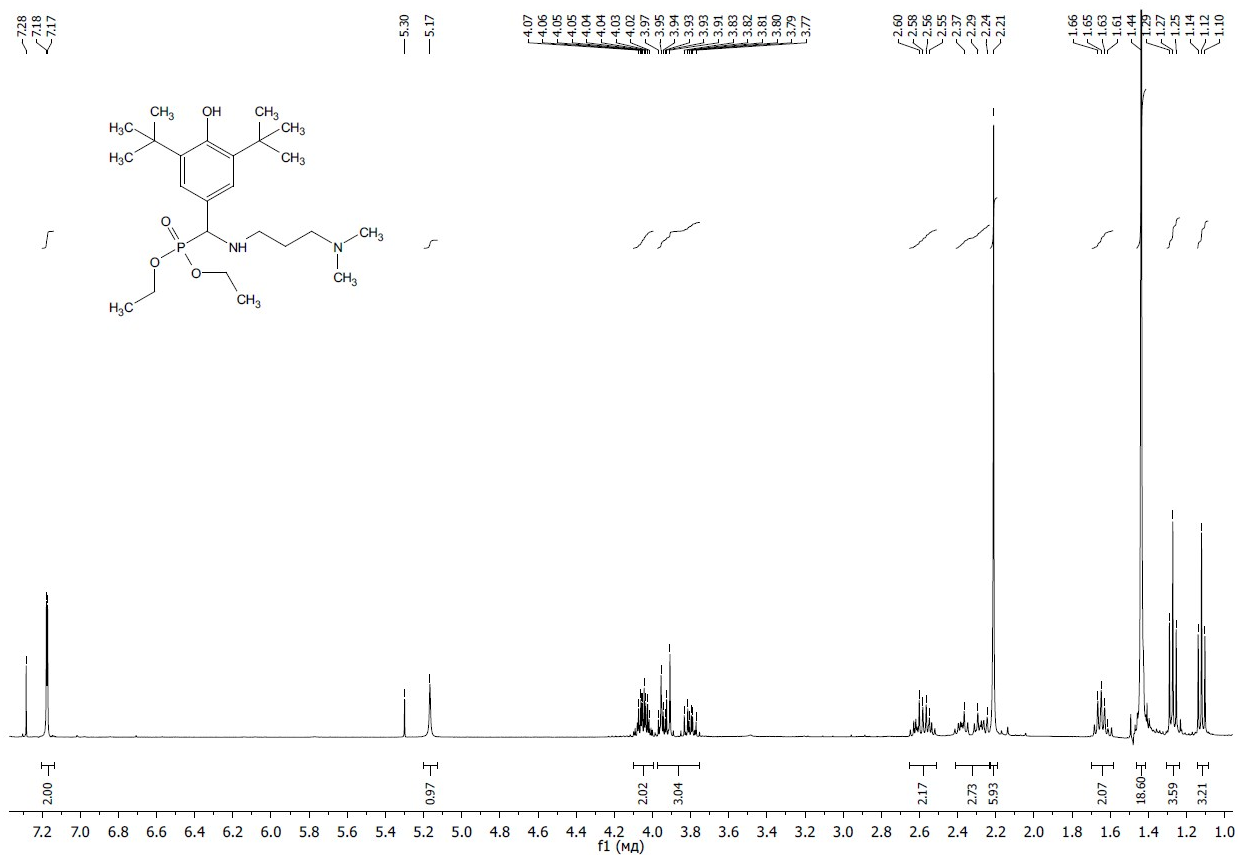
**$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$  NMR spectra compounds 7a and 7b– 16a and 16b** $^1\text{H}$  NMR (CDCl<sub>3</sub>, 400.13 MHz) of 7a



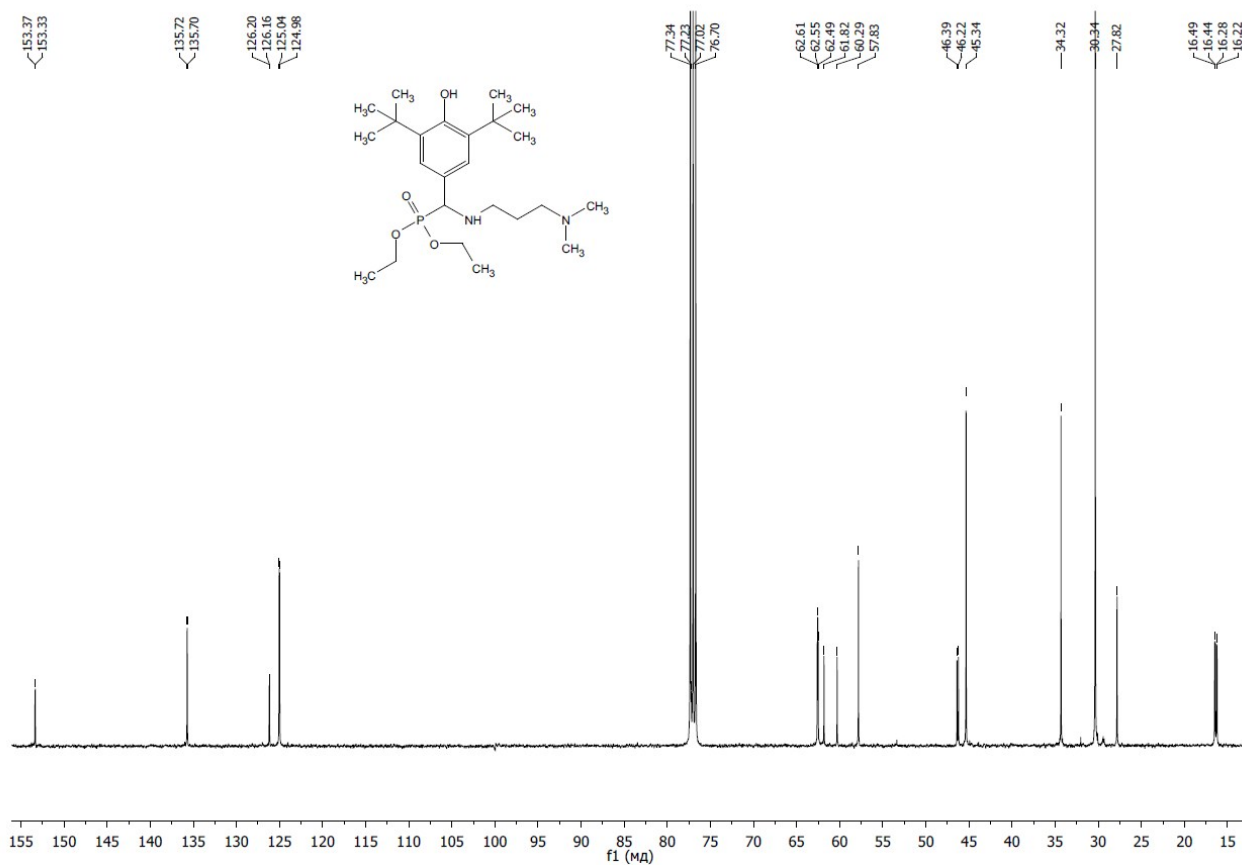
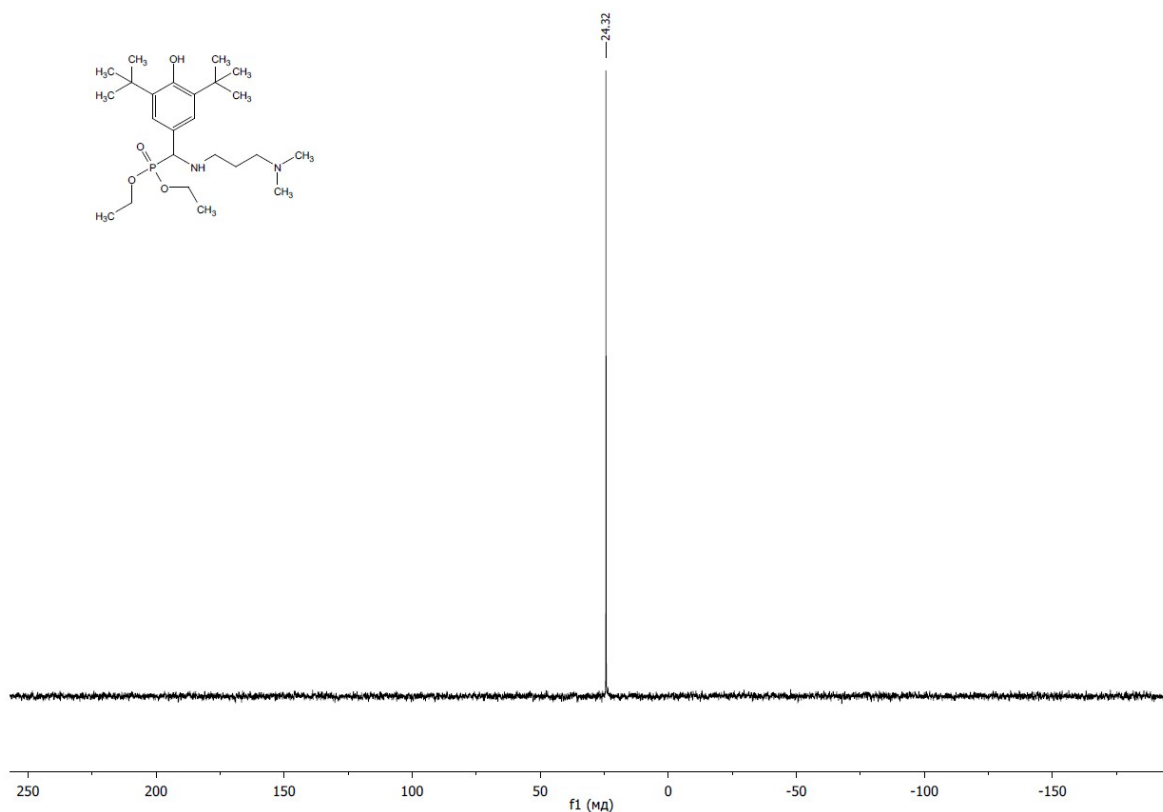
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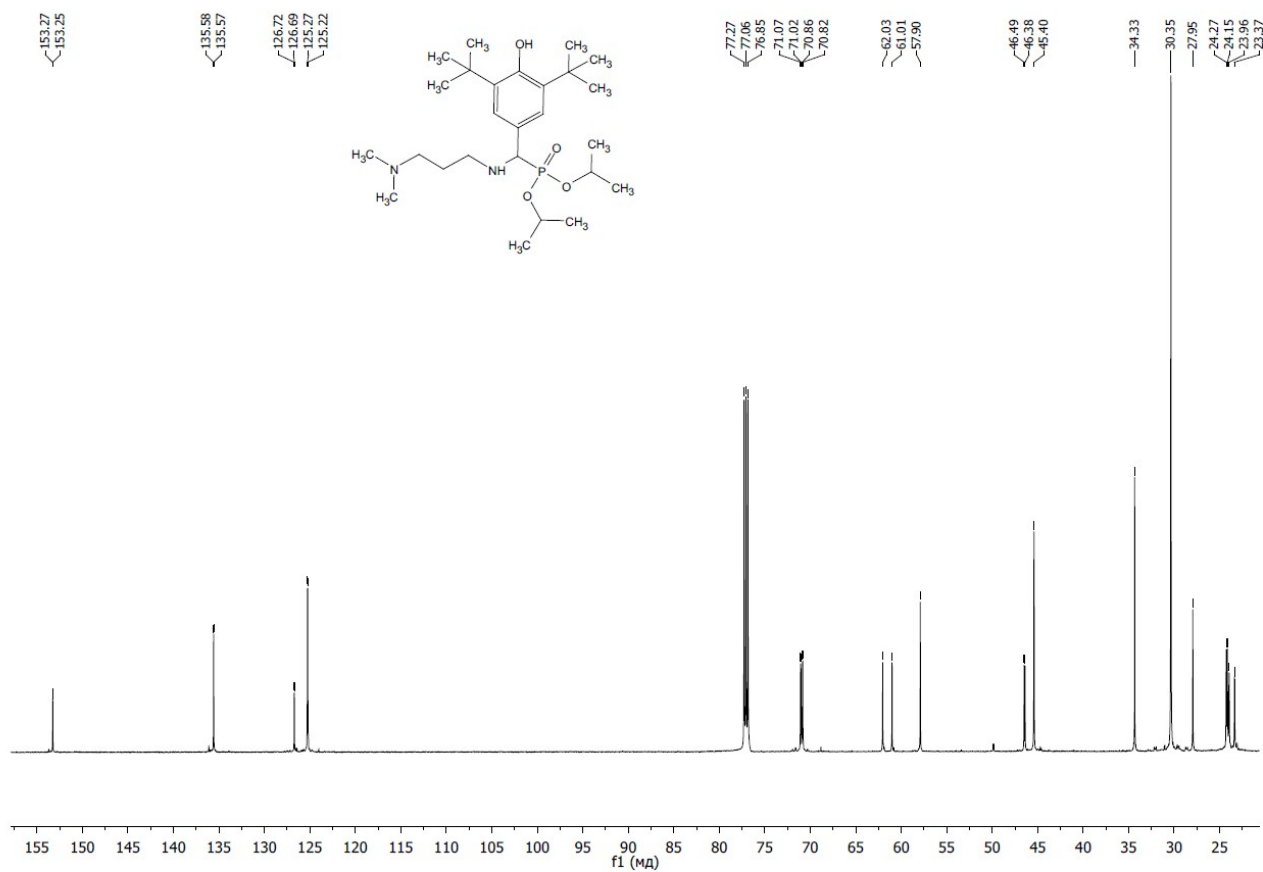
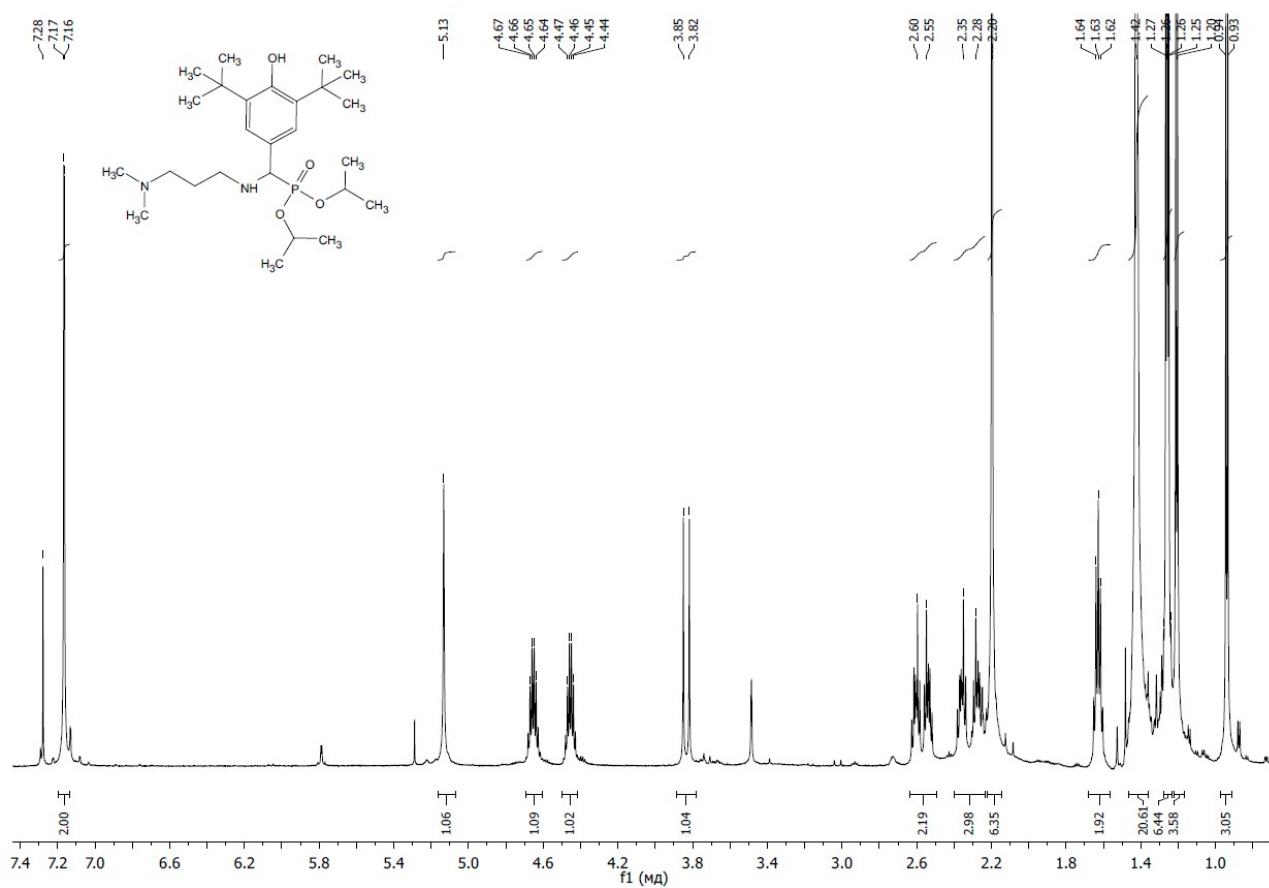


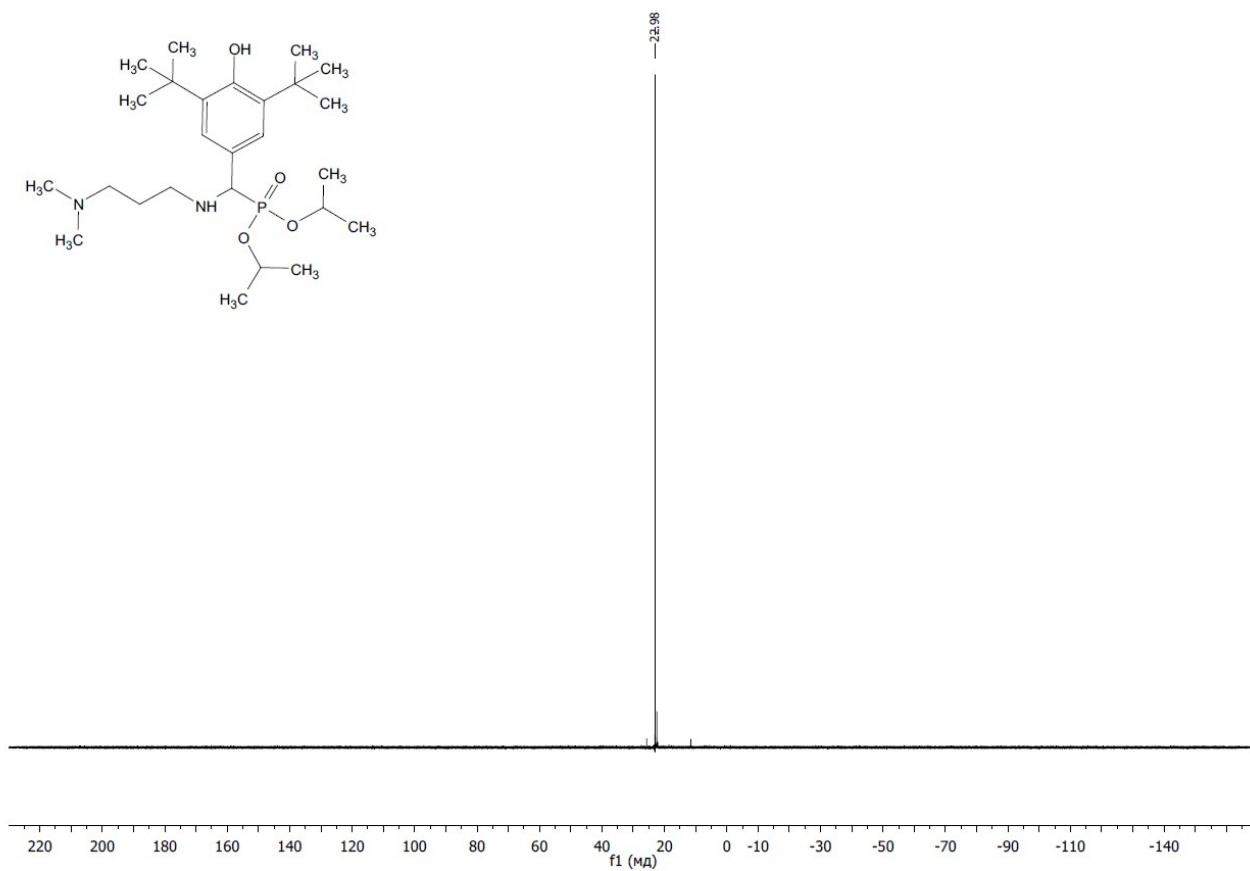
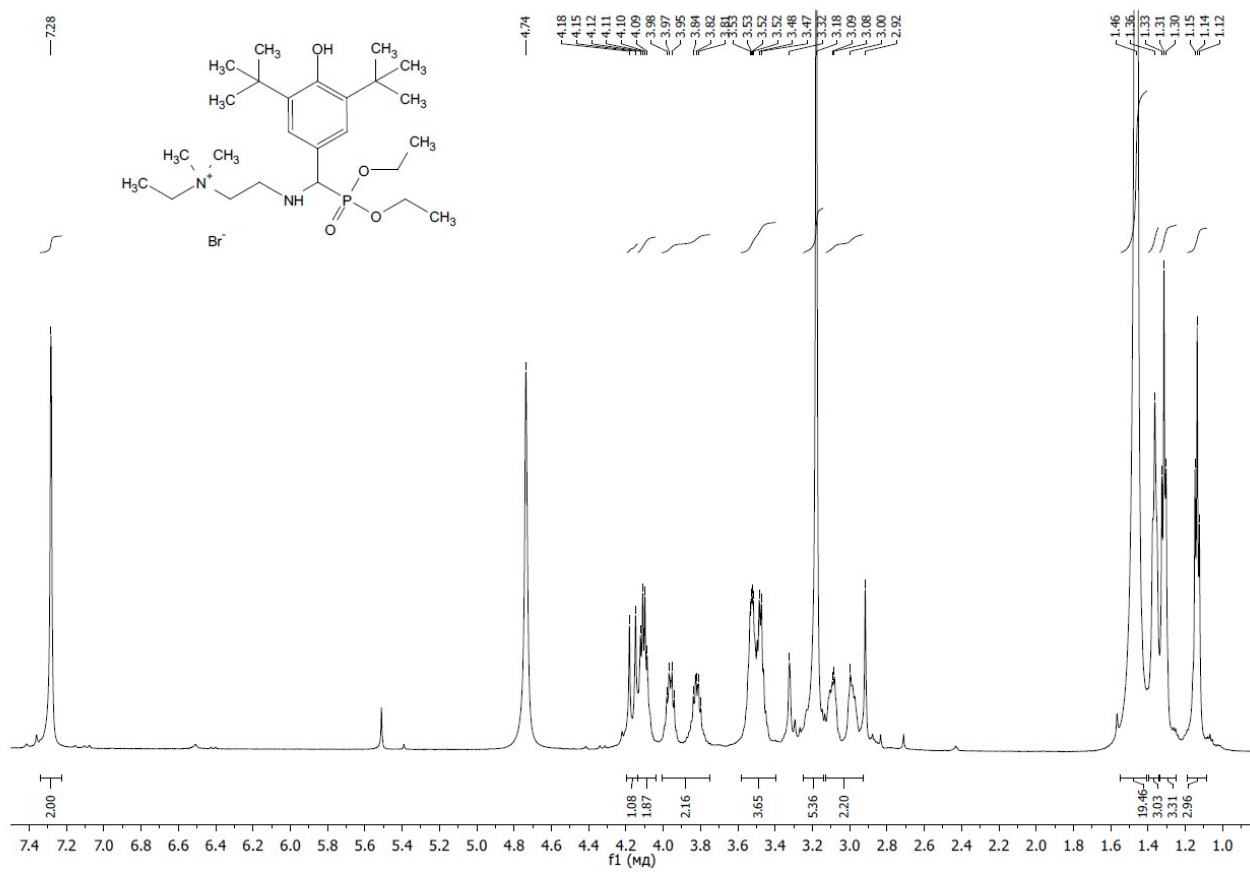
<sup>31</sup>P NMR (CDCl<sub>3</sub>, 161.94 MHz) of 7a<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400.13 MHz) of 7b

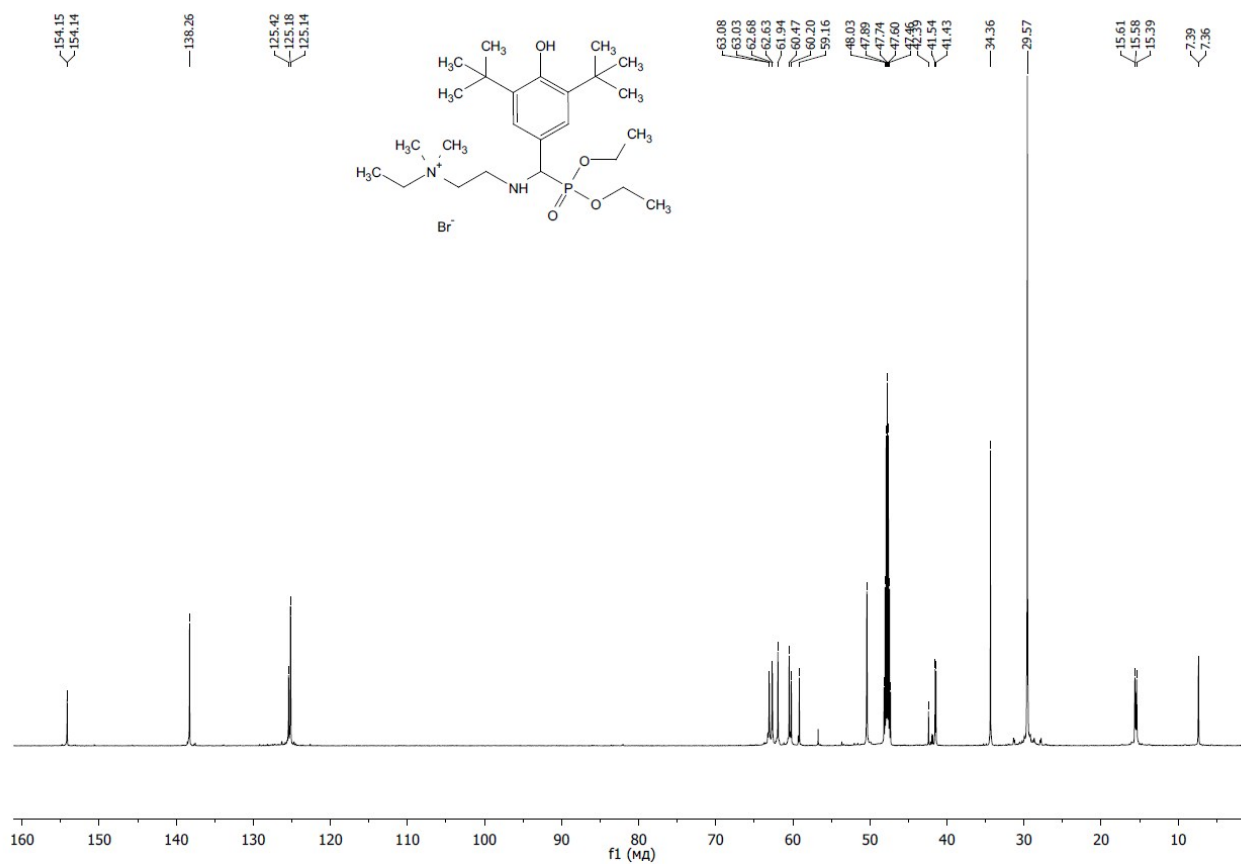
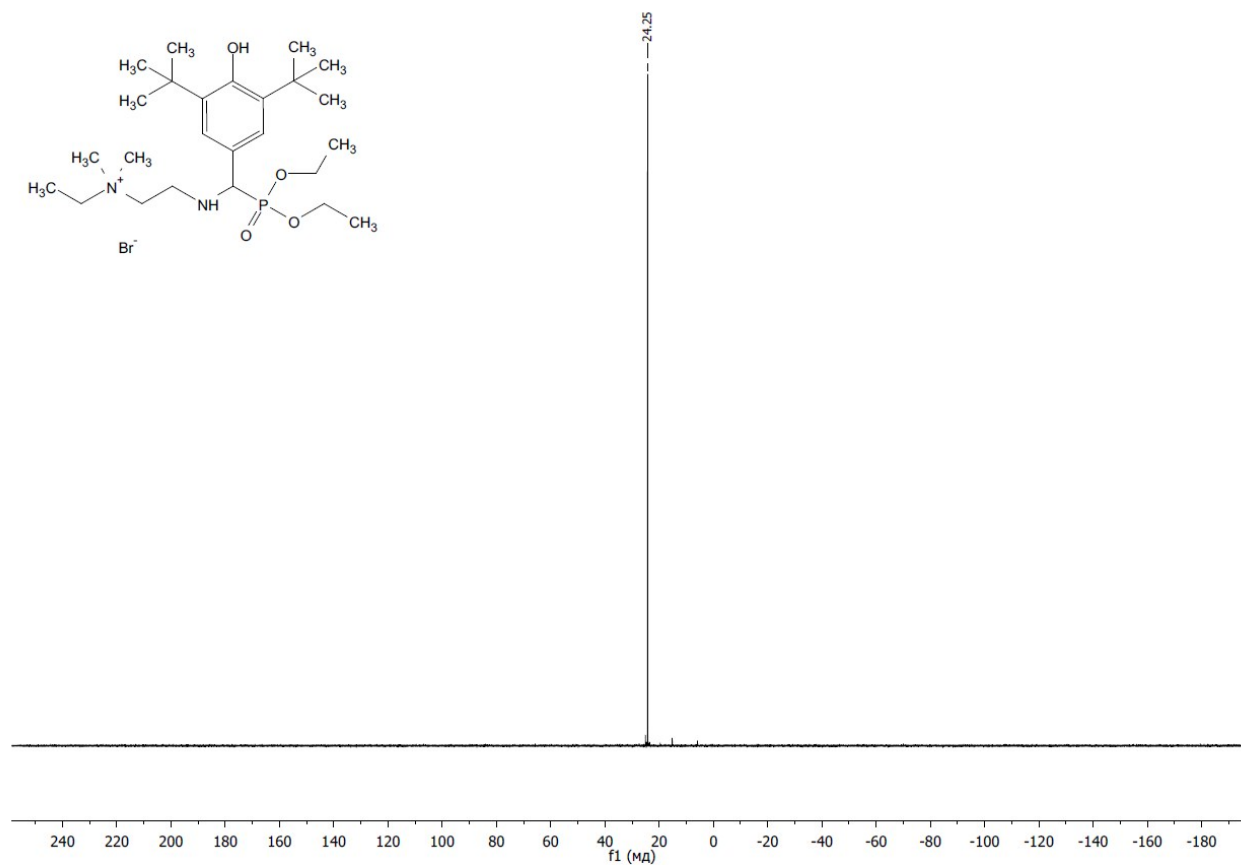
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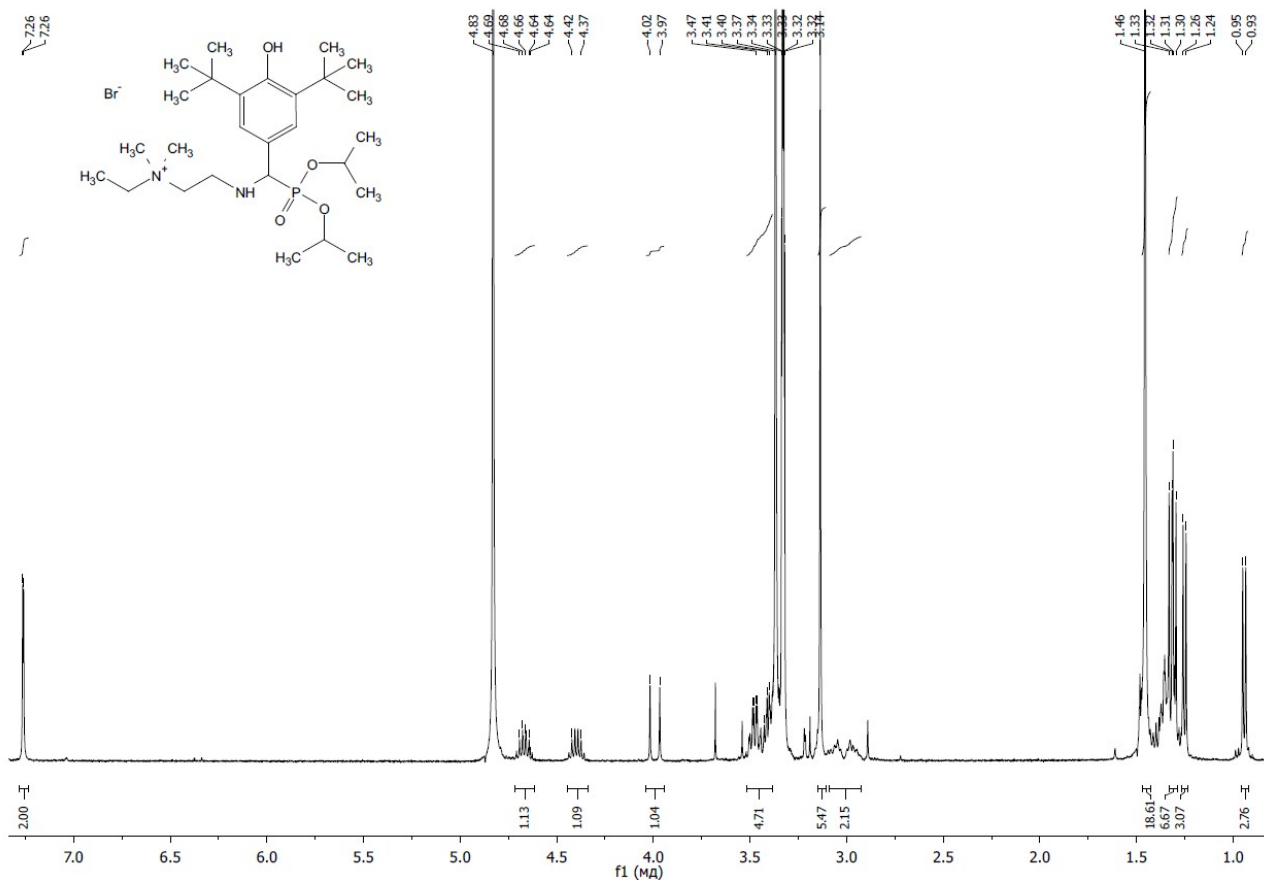


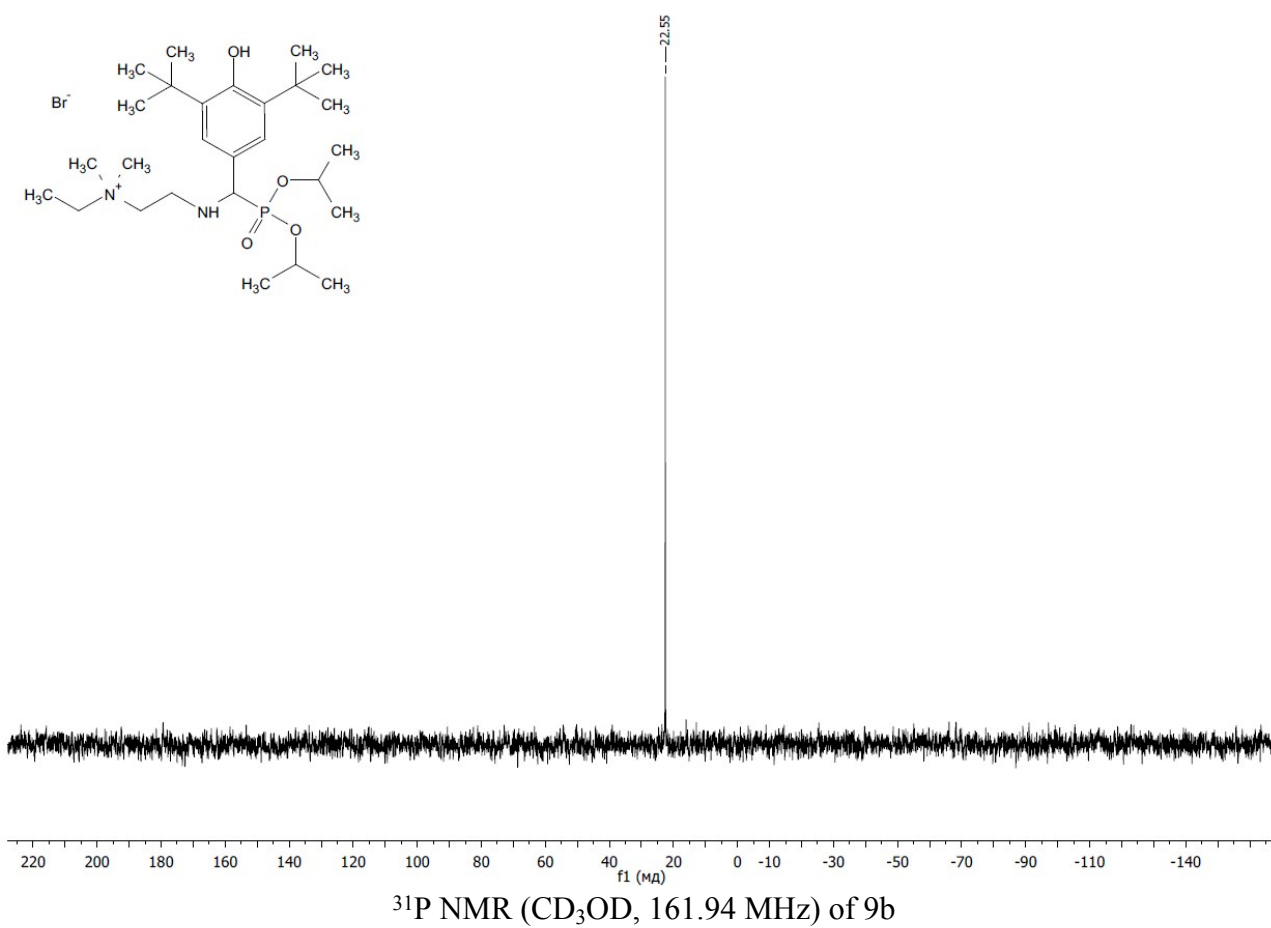
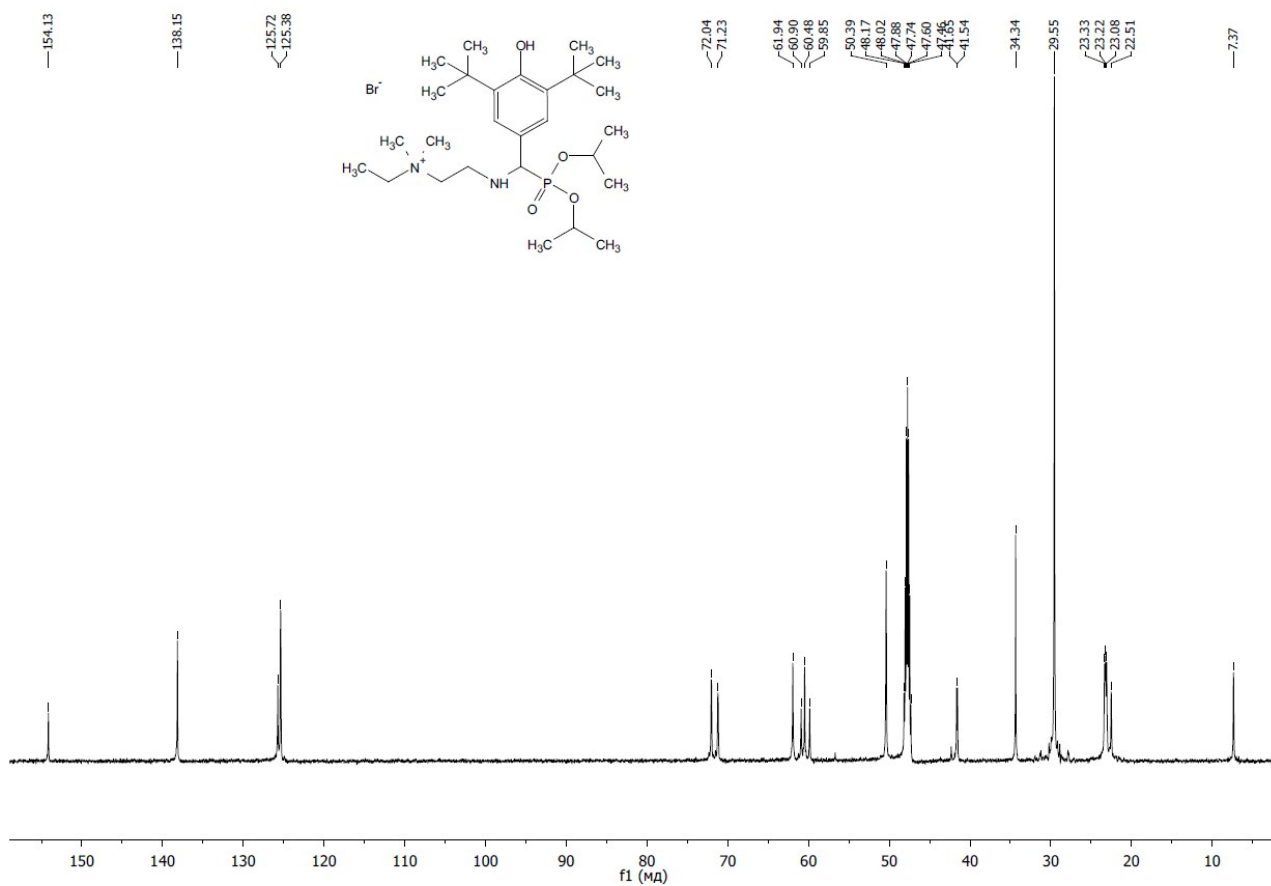
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400.13 MHz) of 8a $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz) of 8a $^{31}\text{P}$  NMR ( $\text{CDCl}_3$ , 161.94 MHz) of 8a

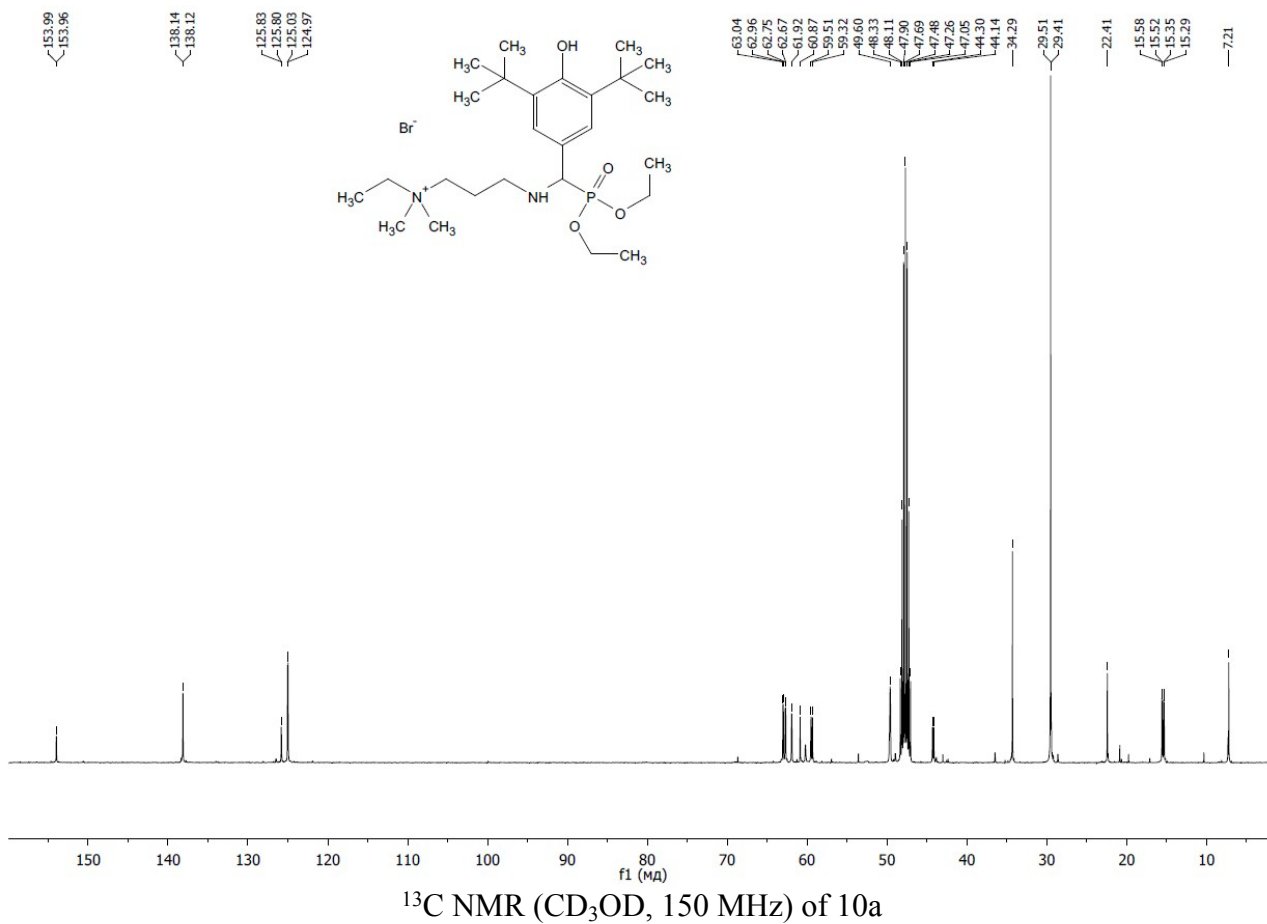
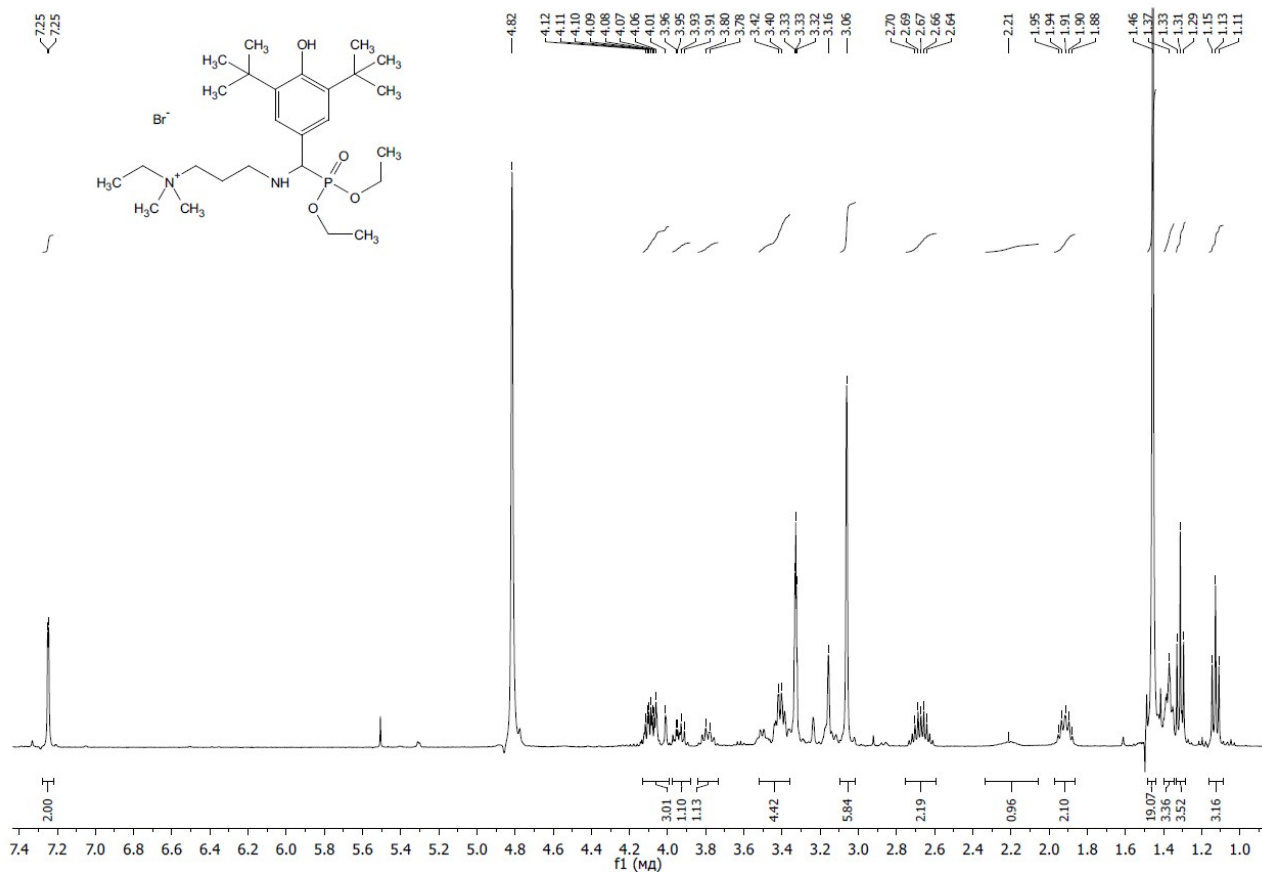


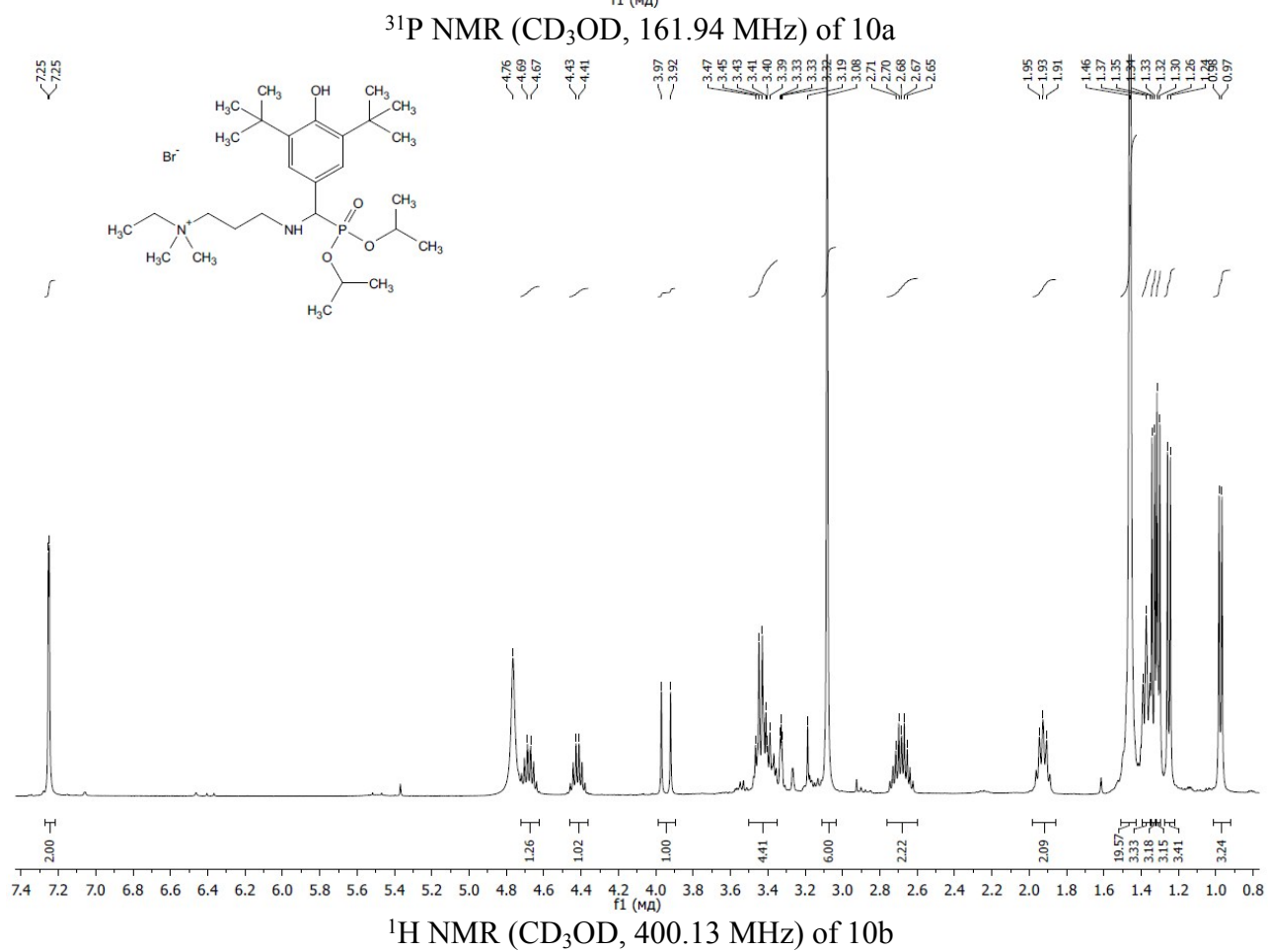
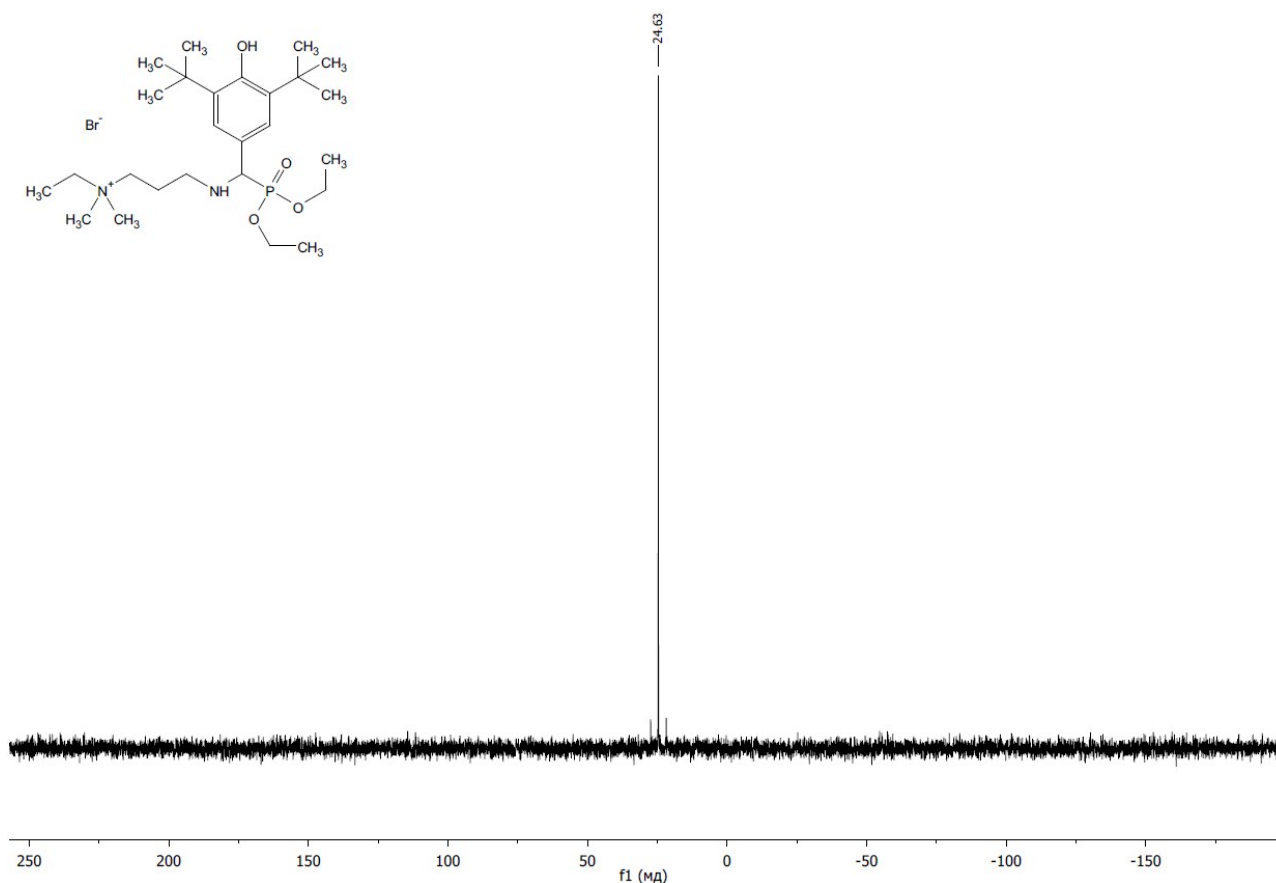
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$^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400.13 MHz) of 9a $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 150 MHz) of 9a

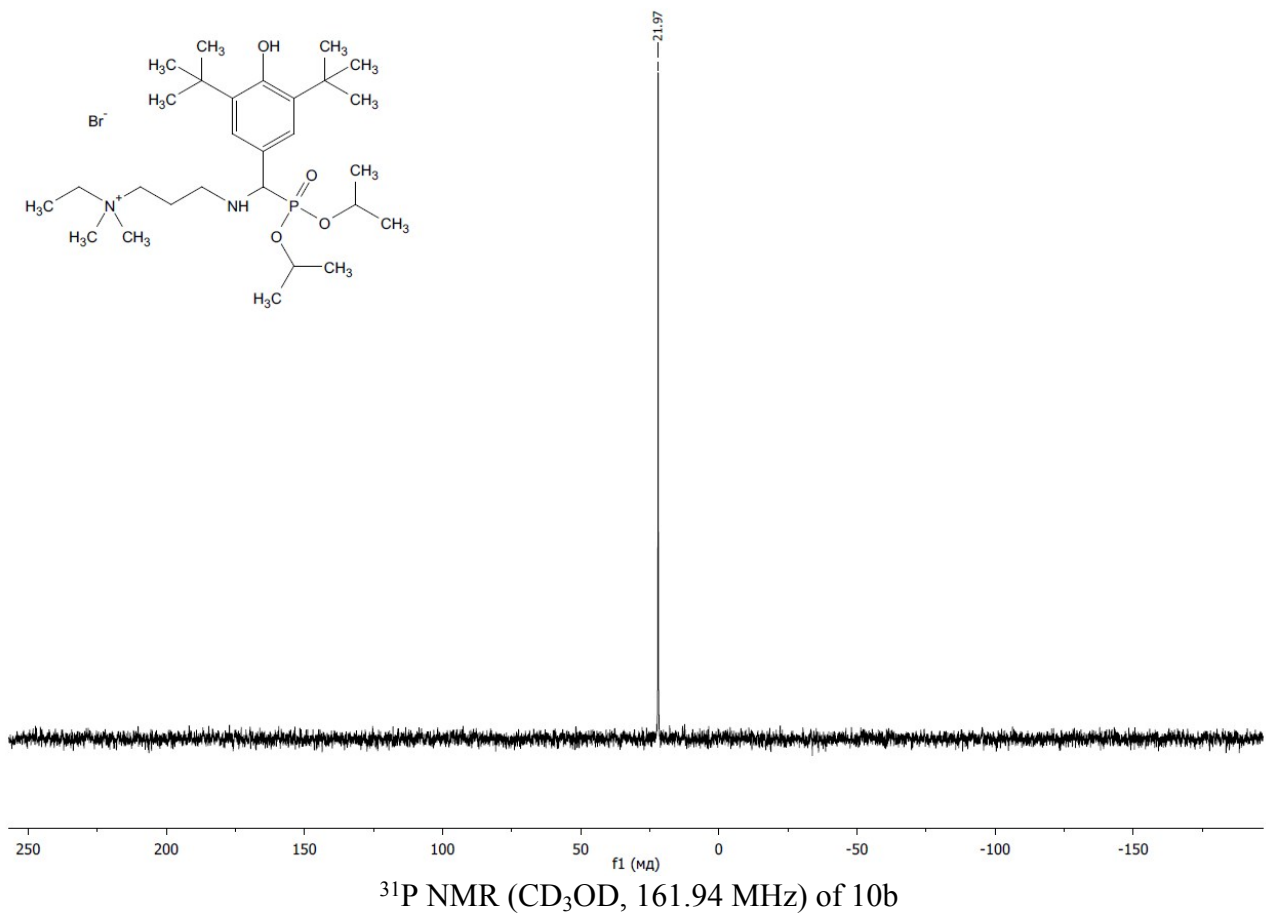
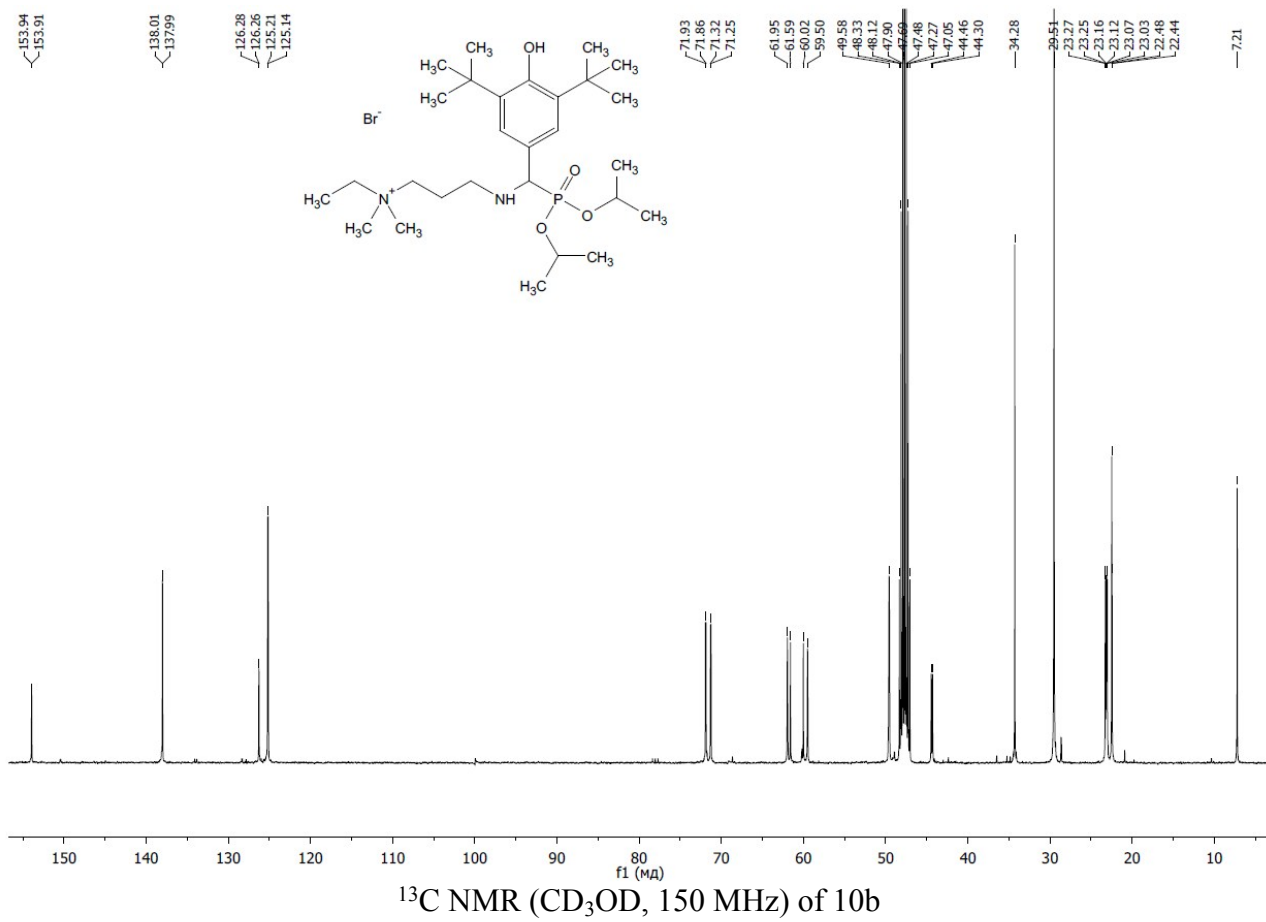
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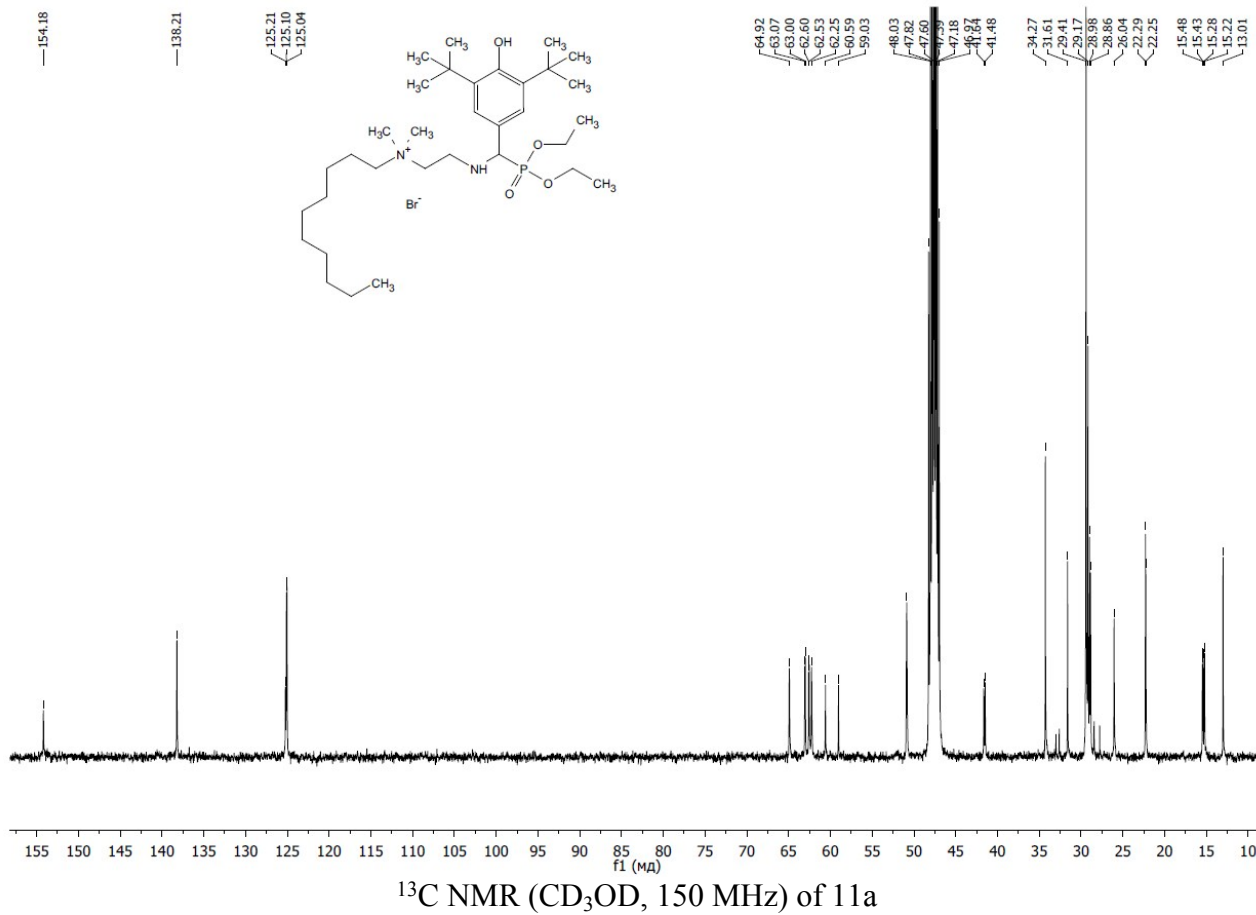
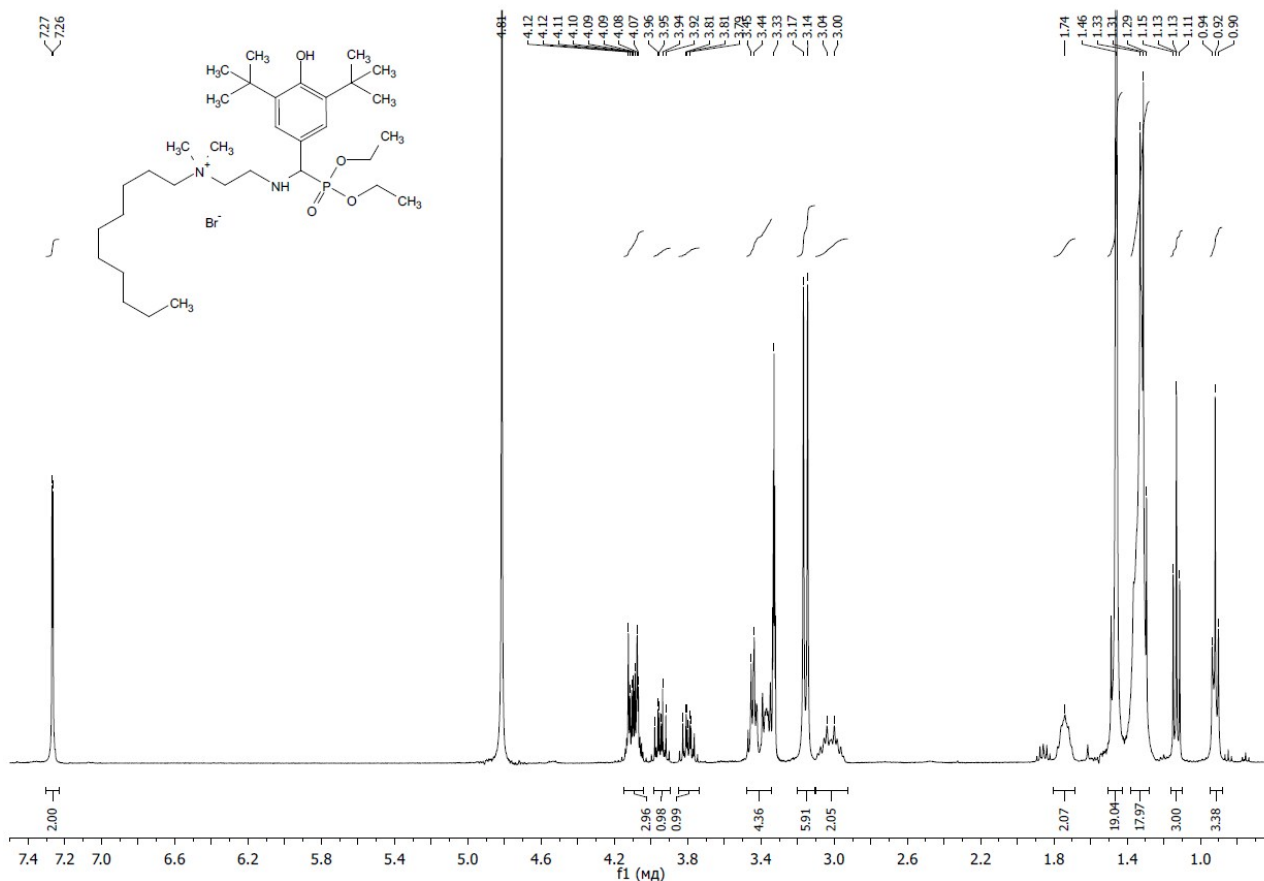


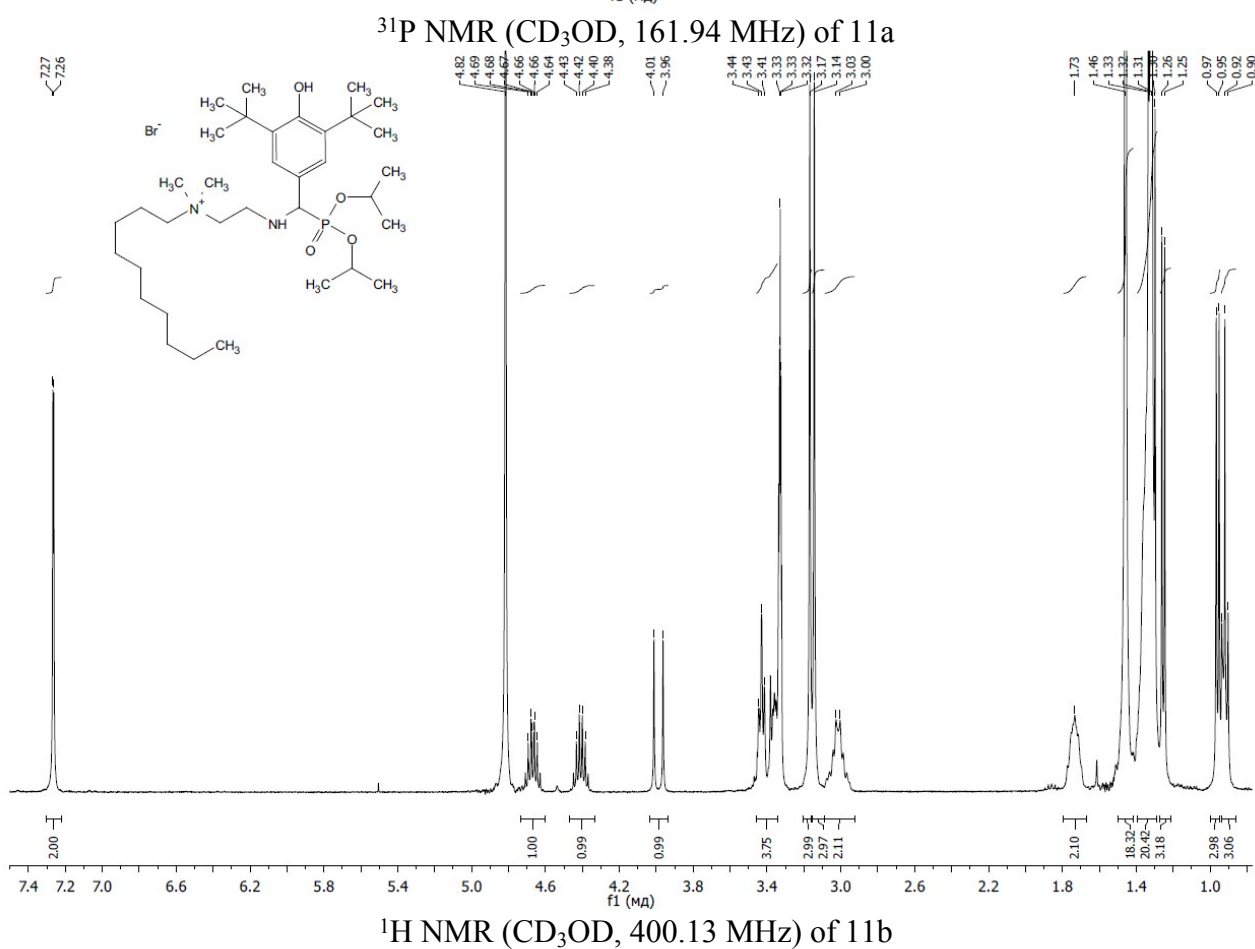
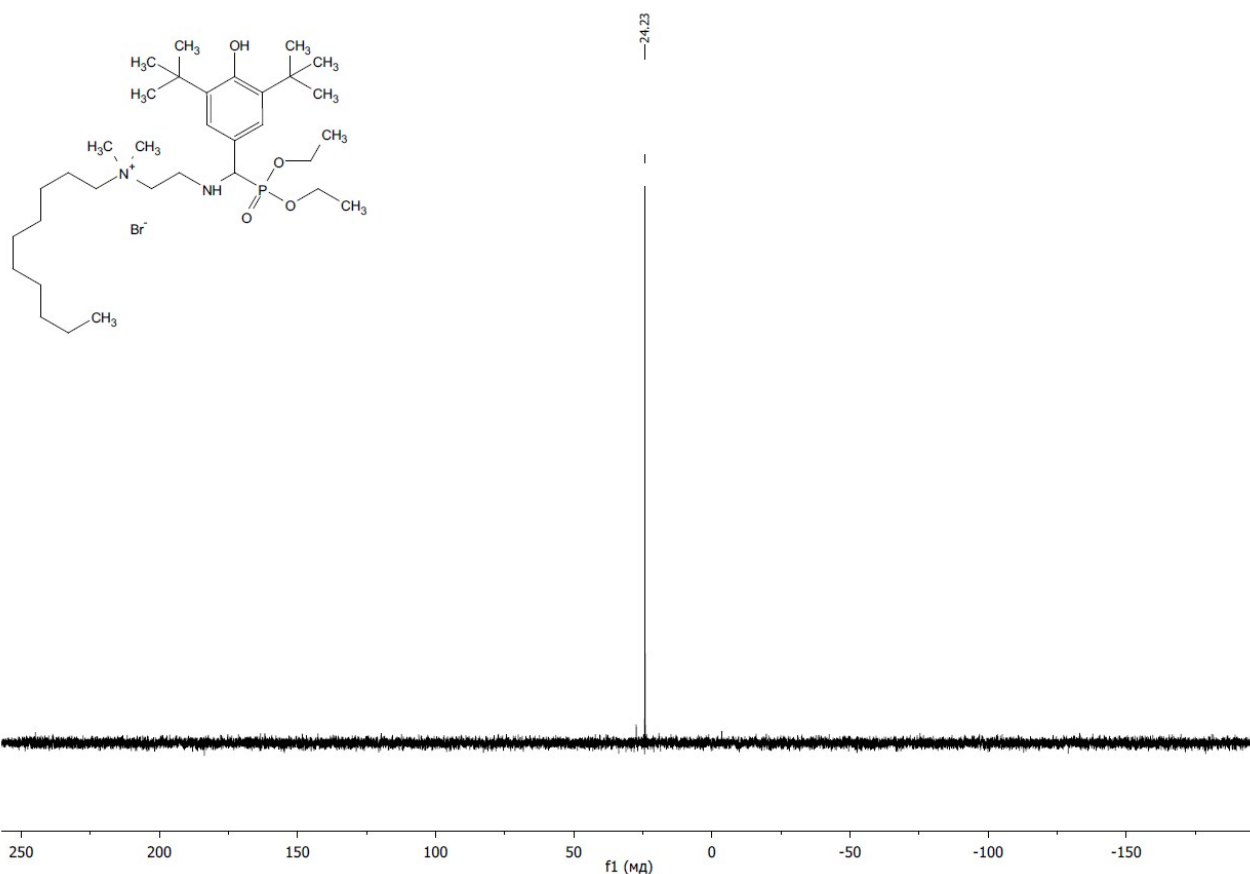


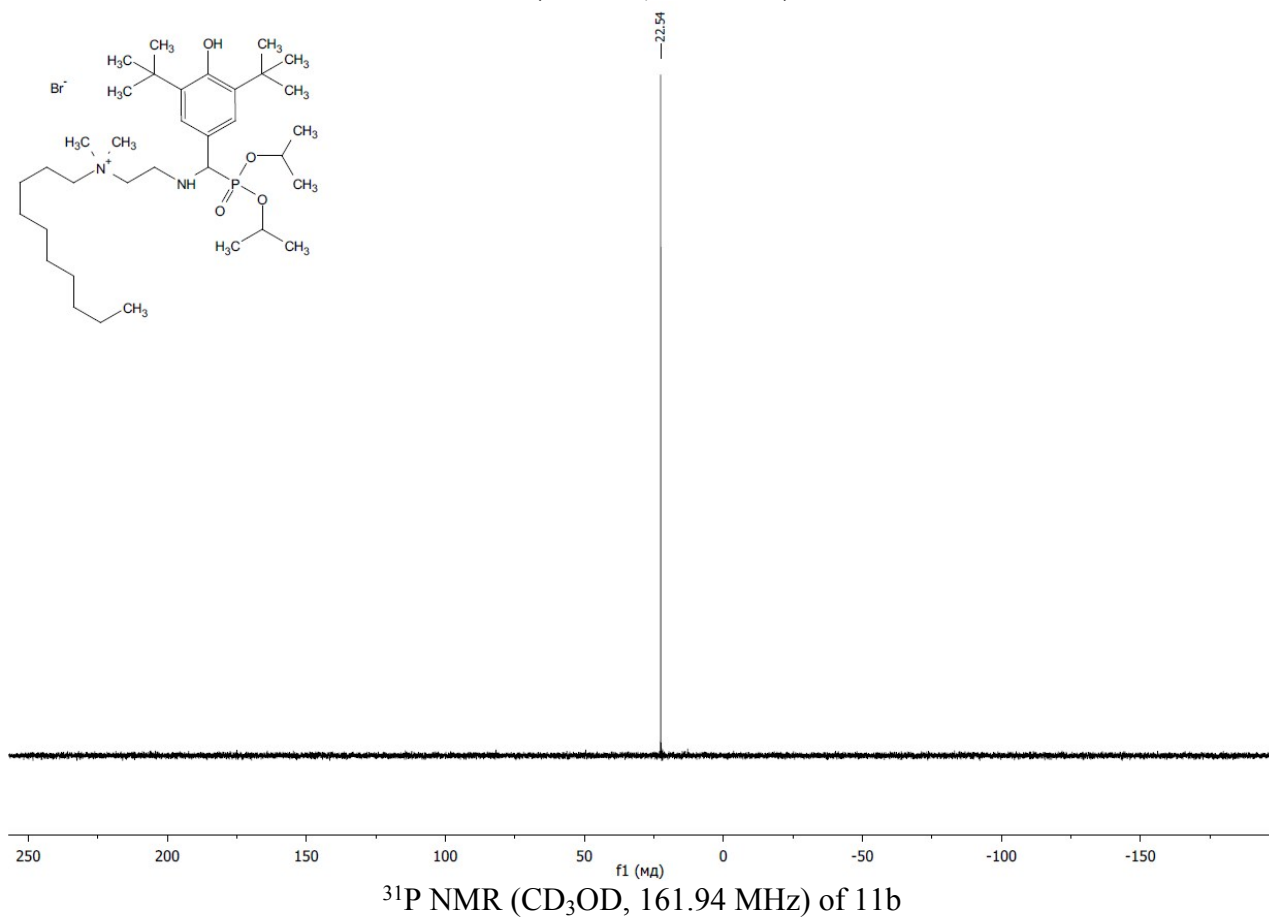
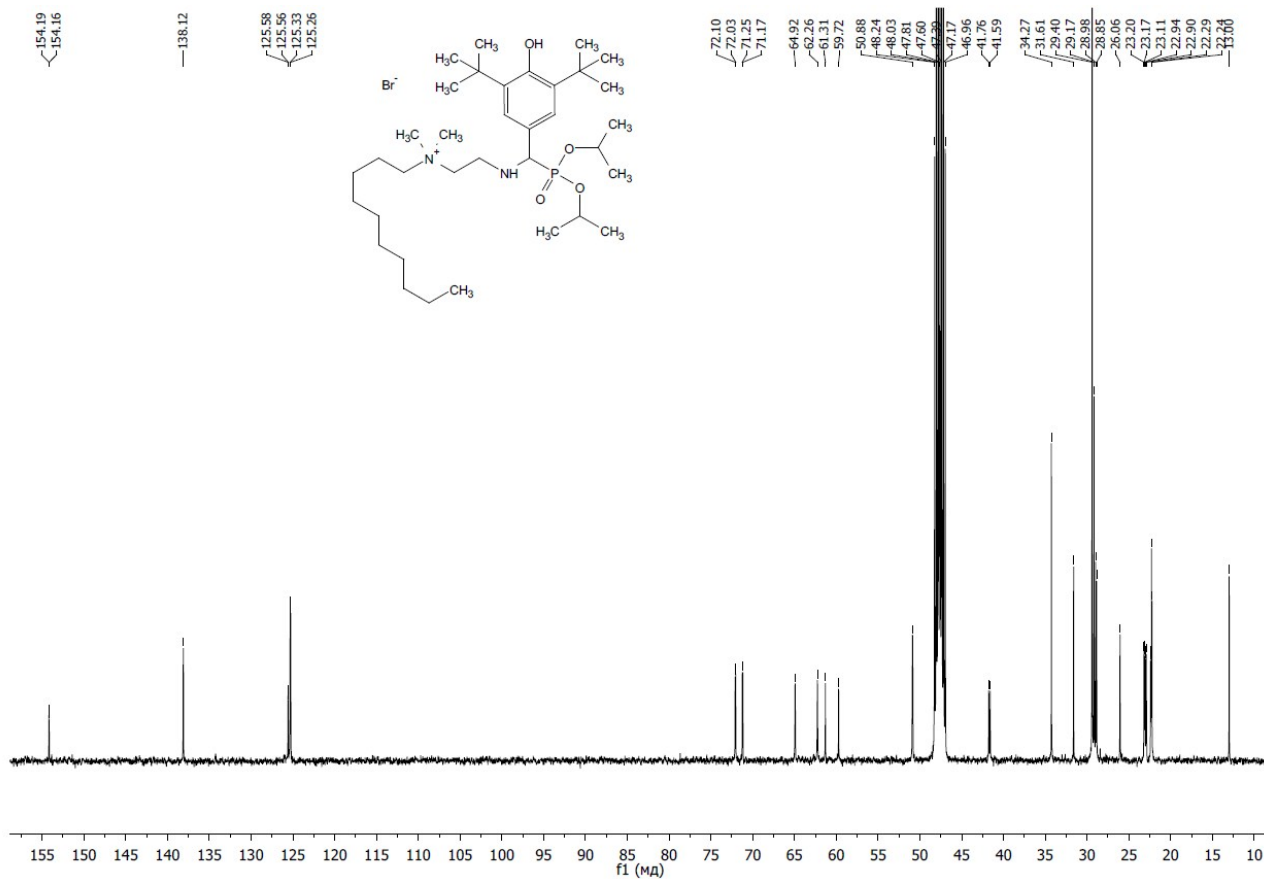


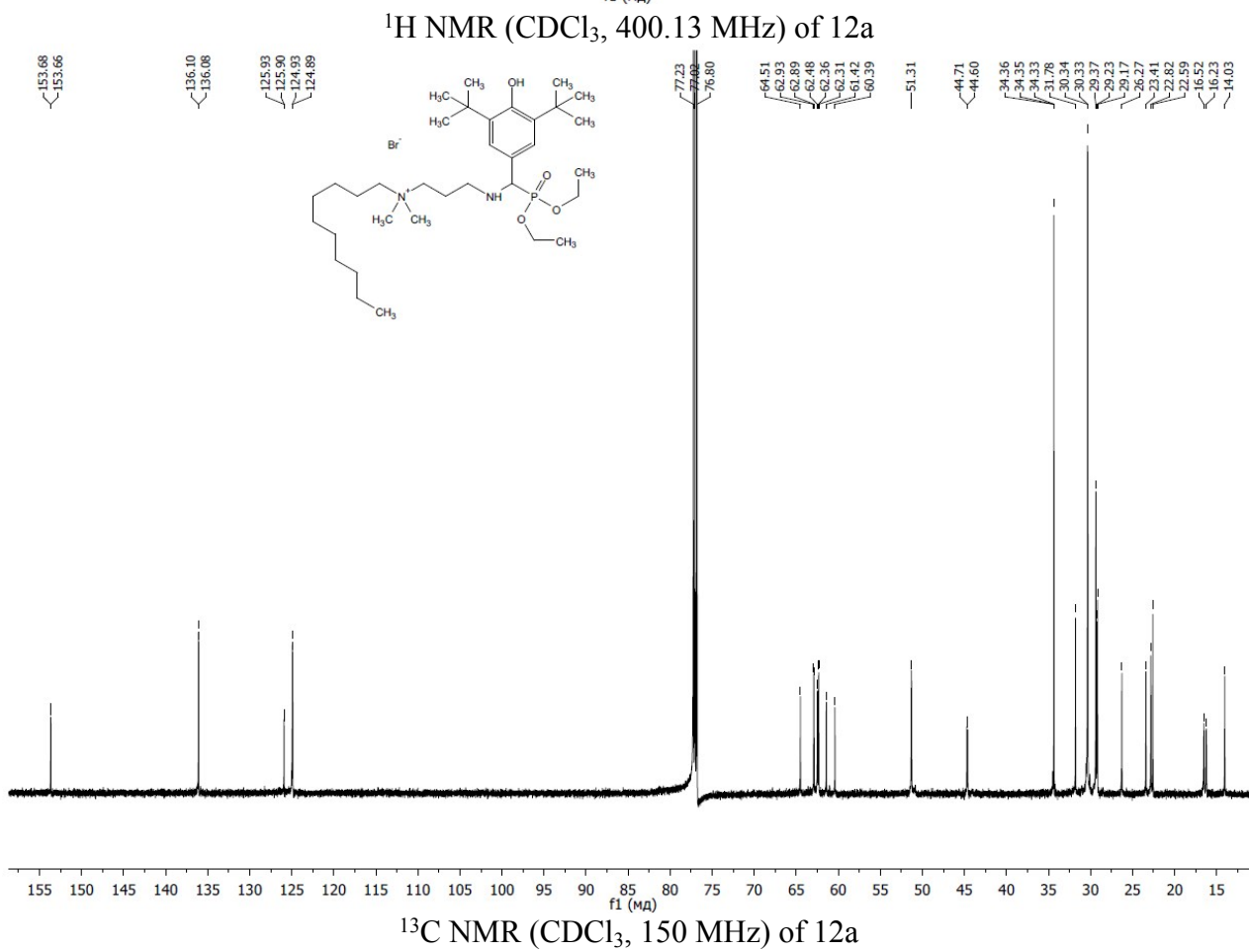
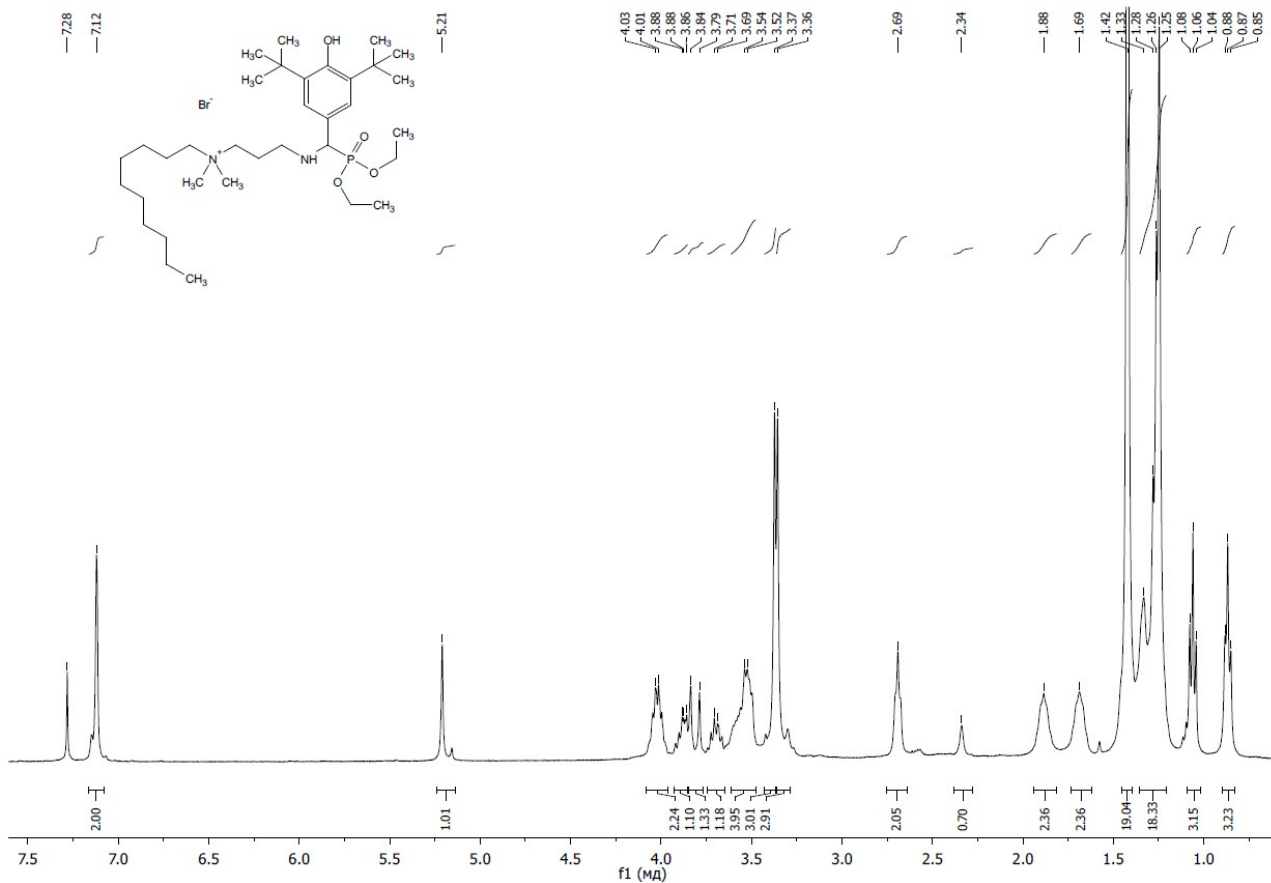


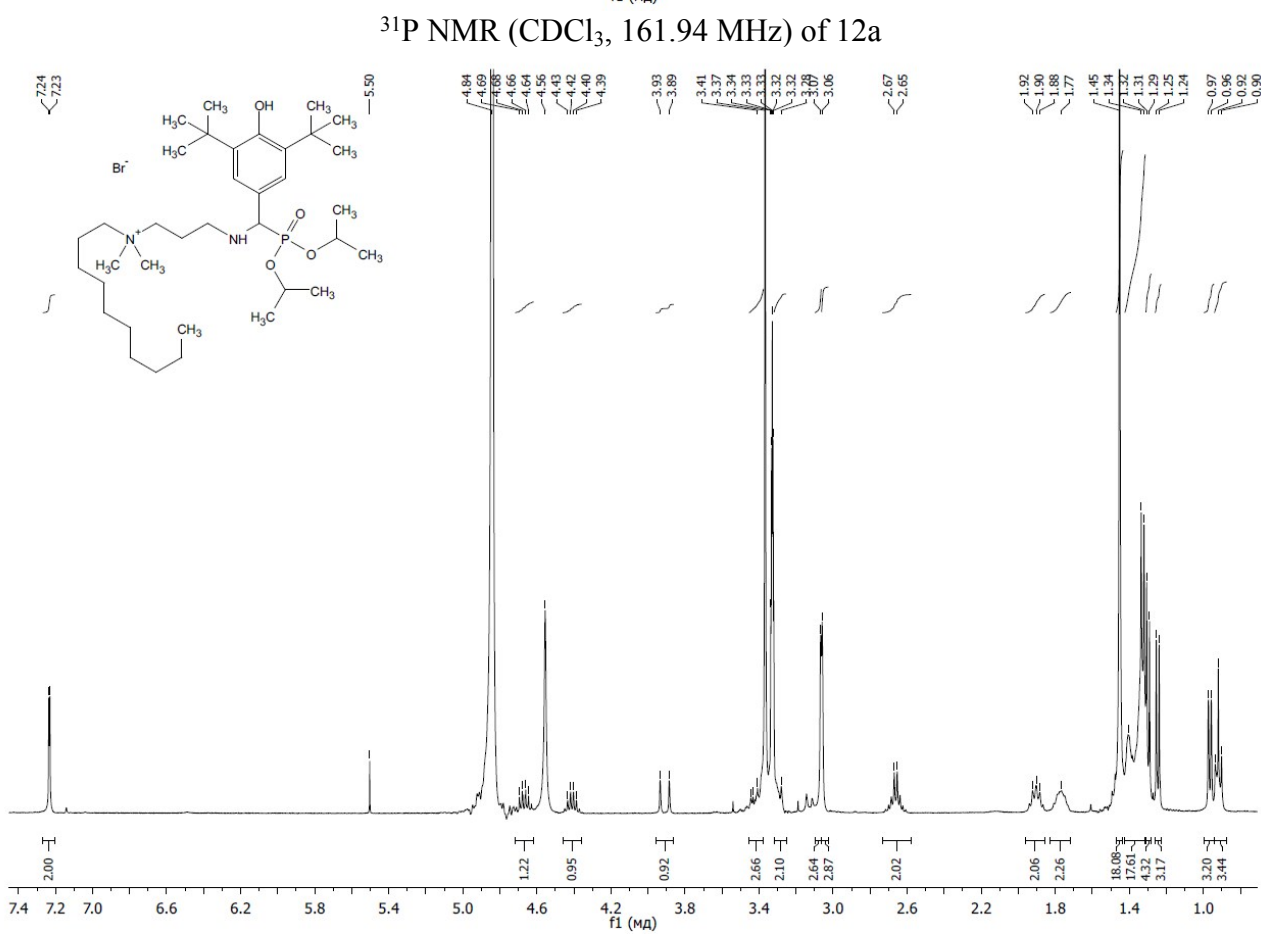
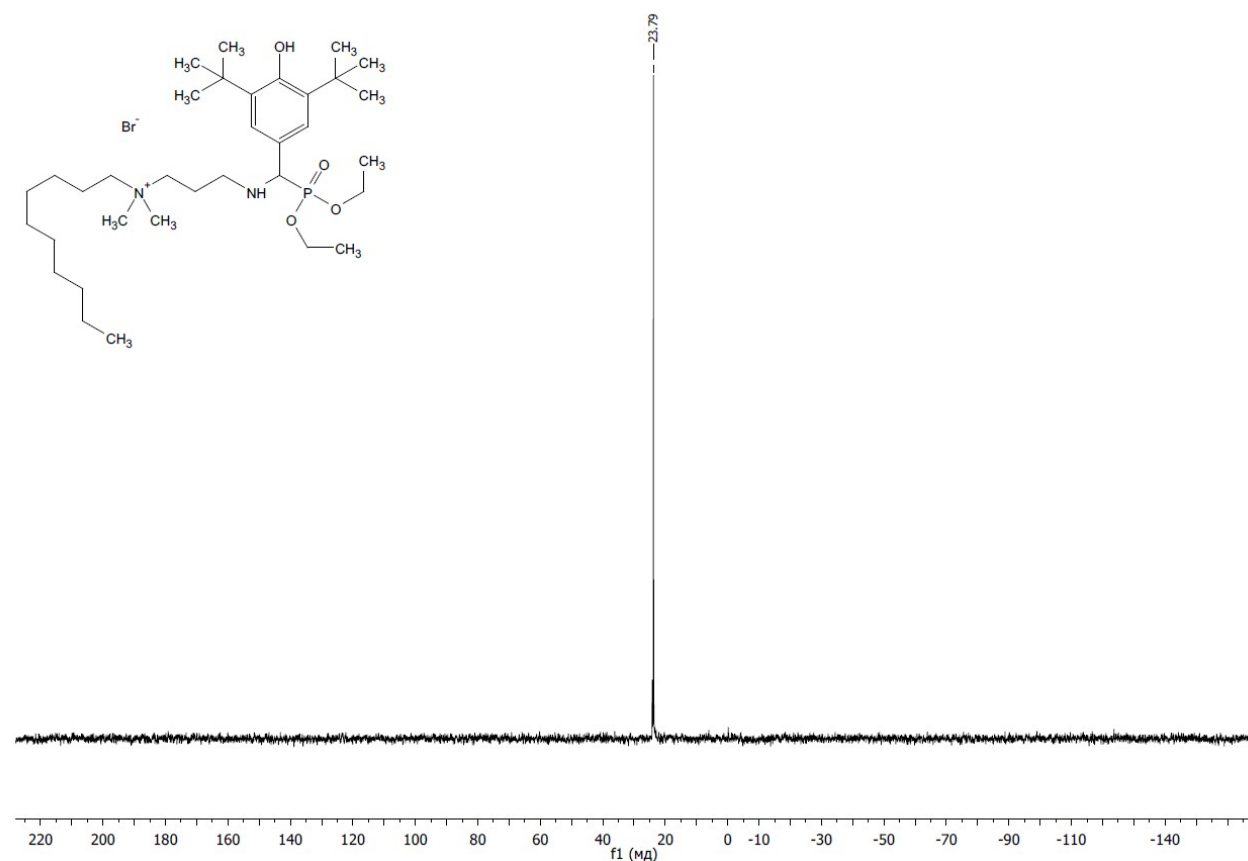


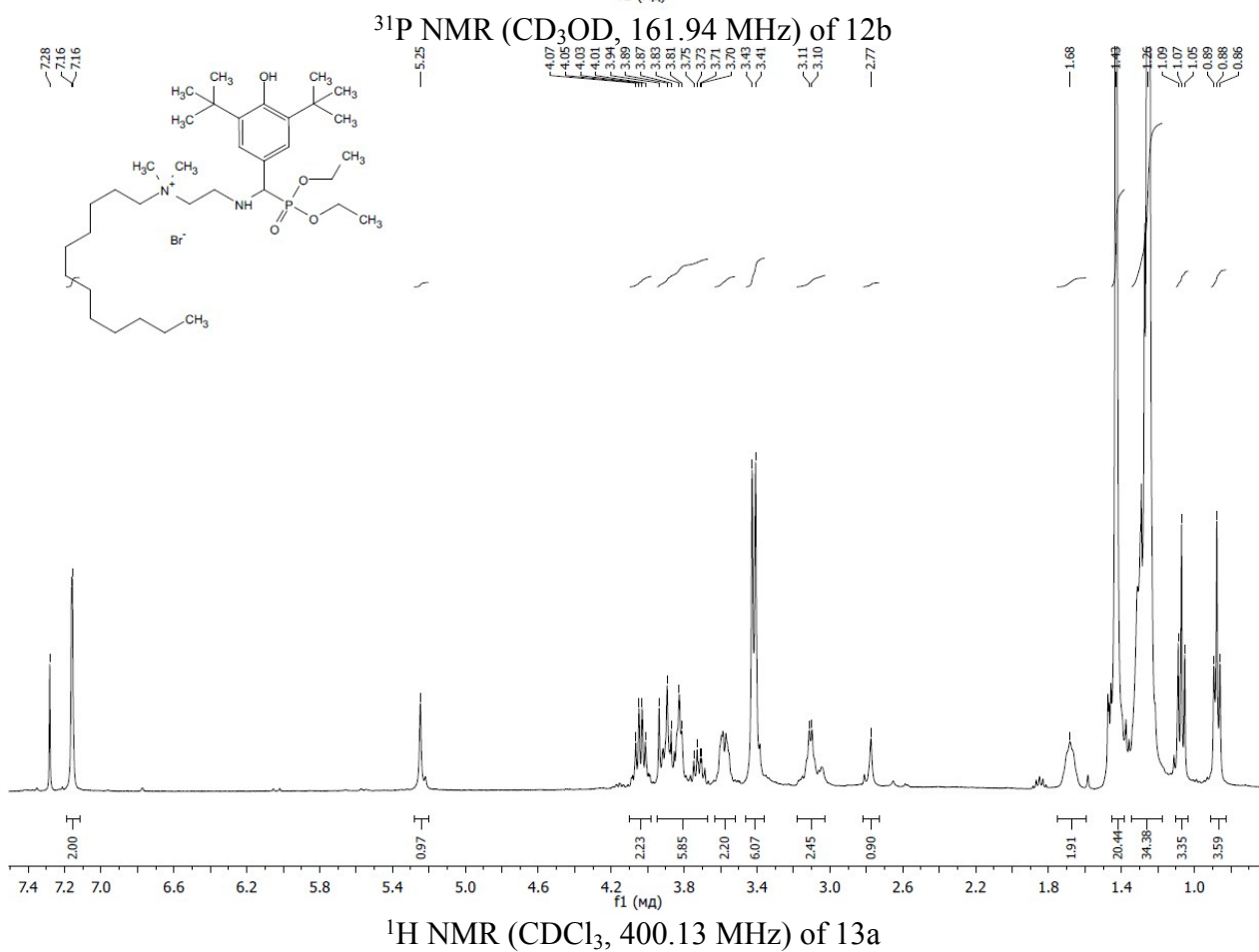
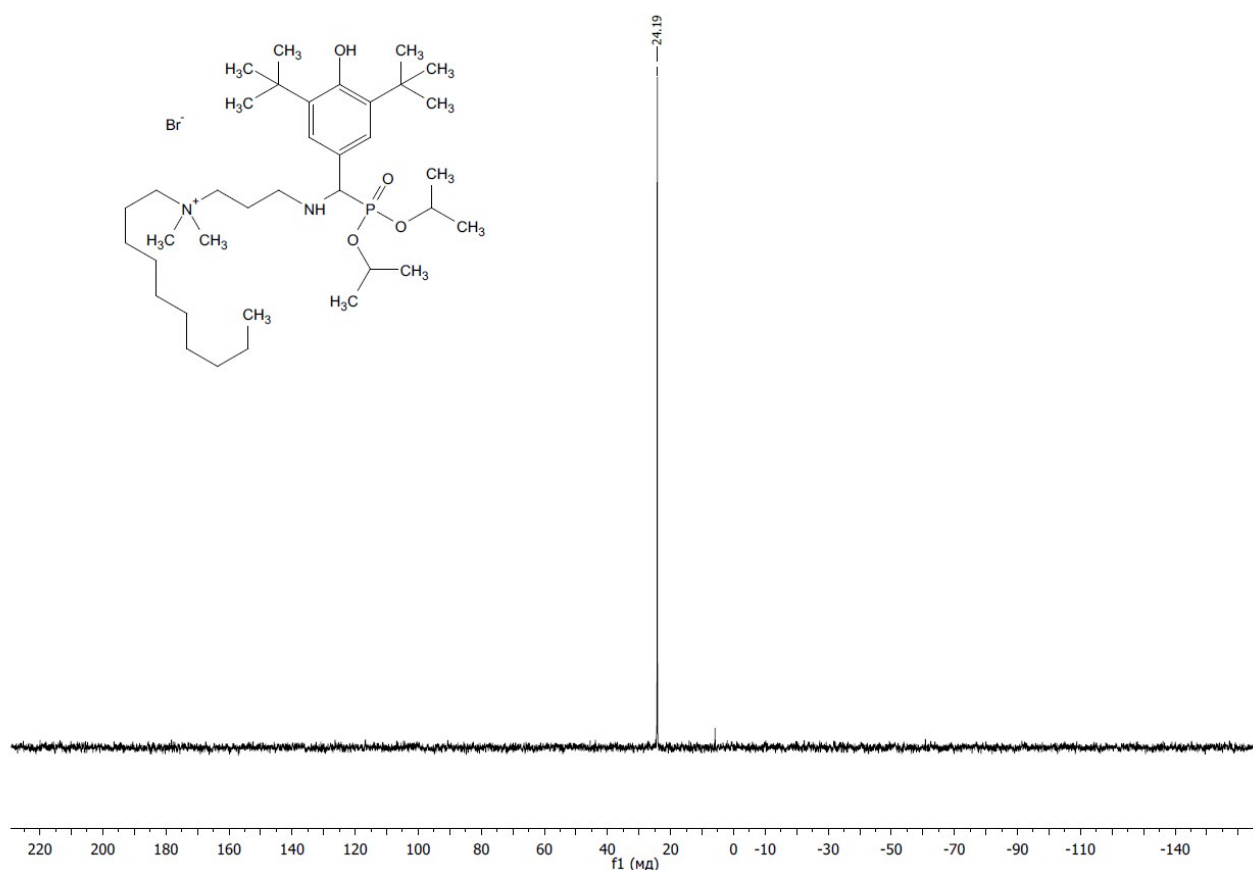


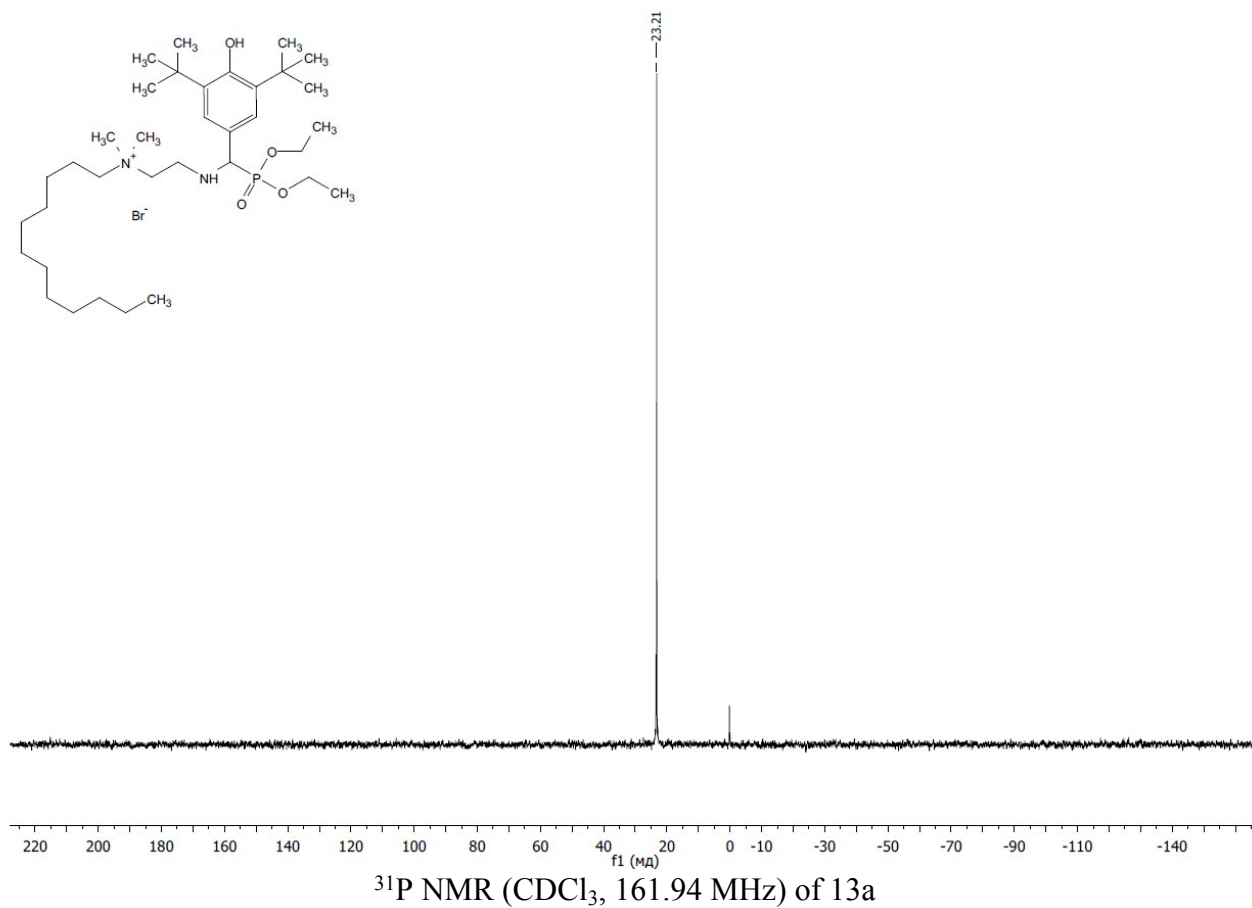
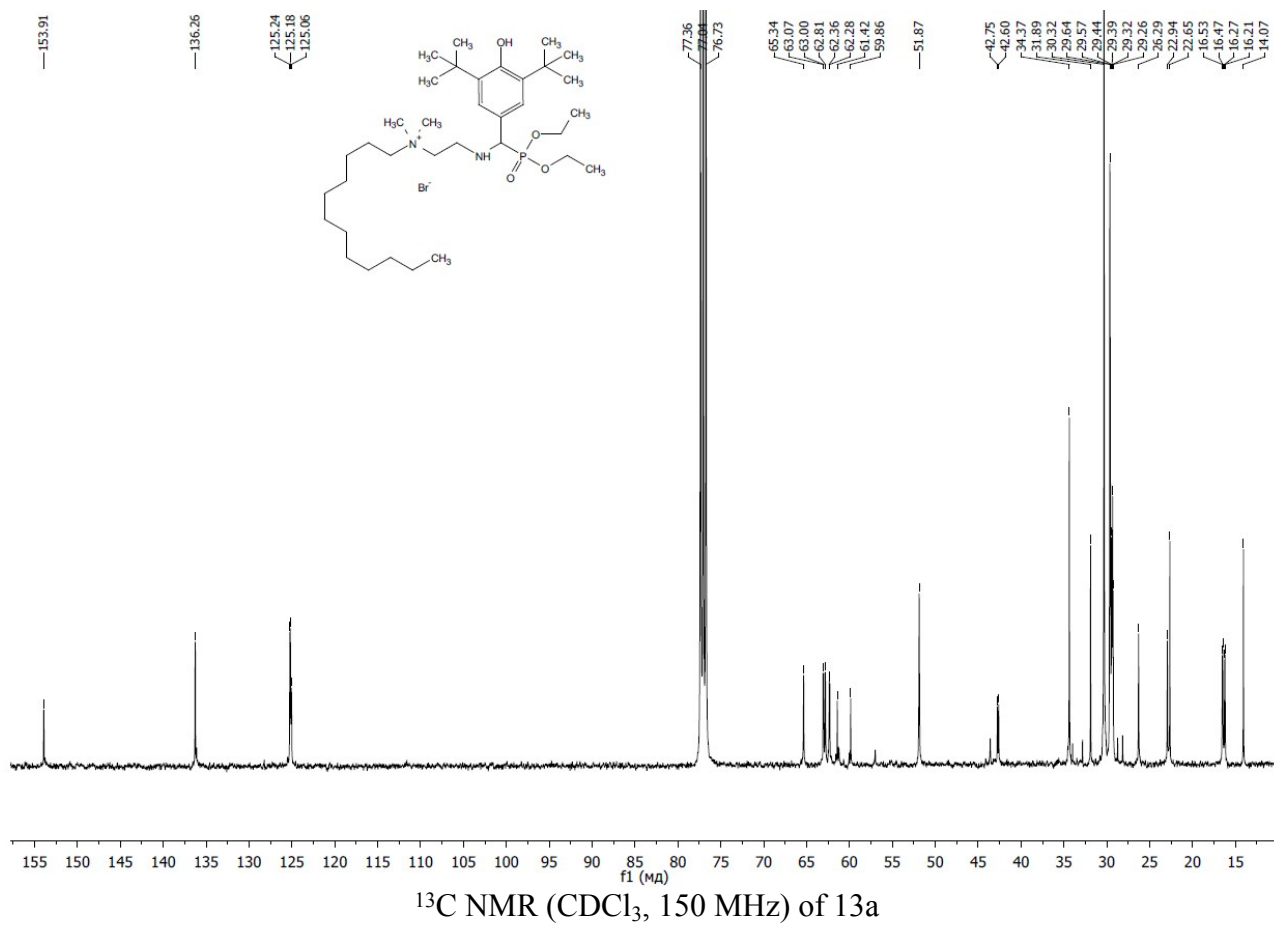




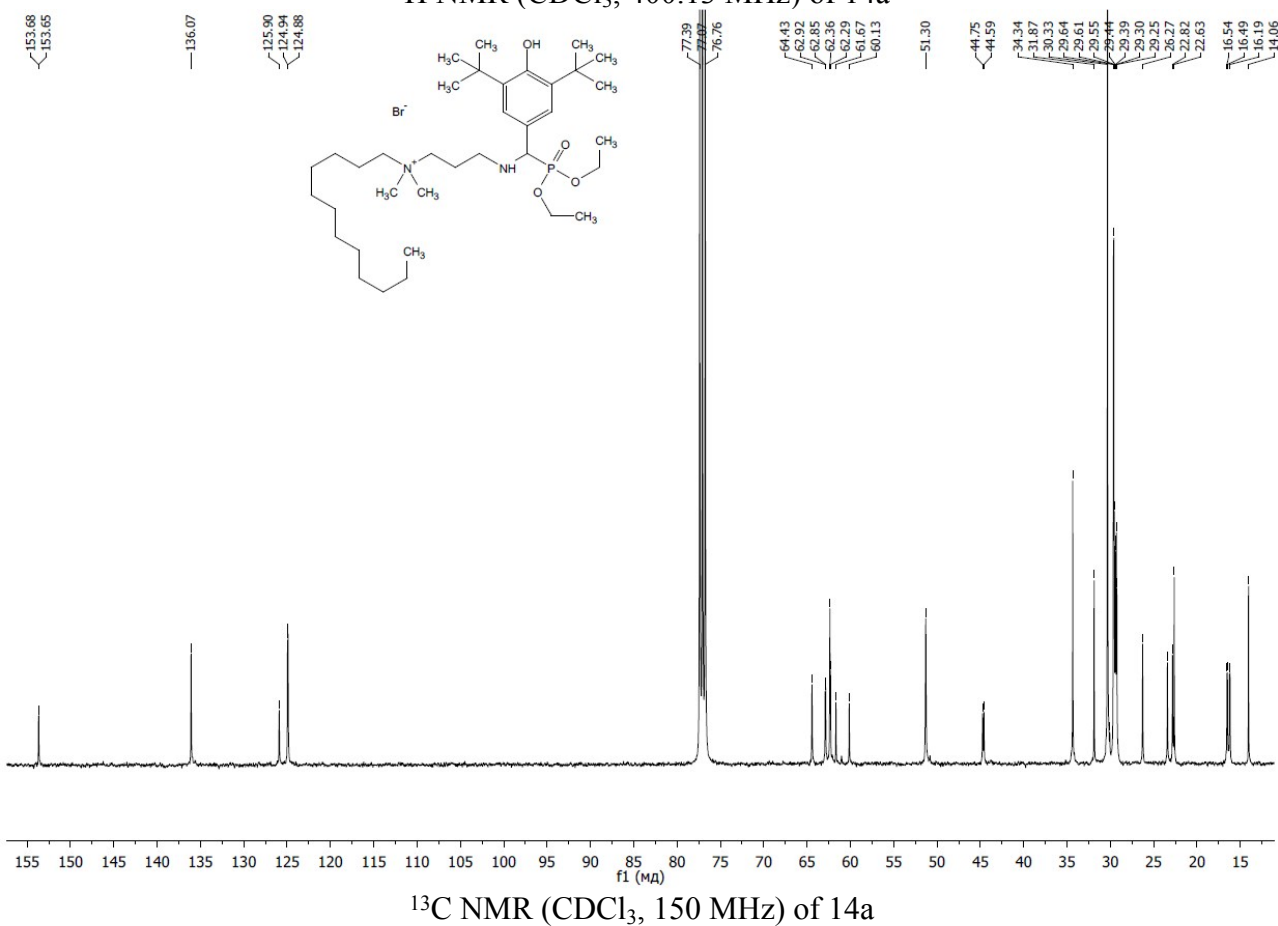
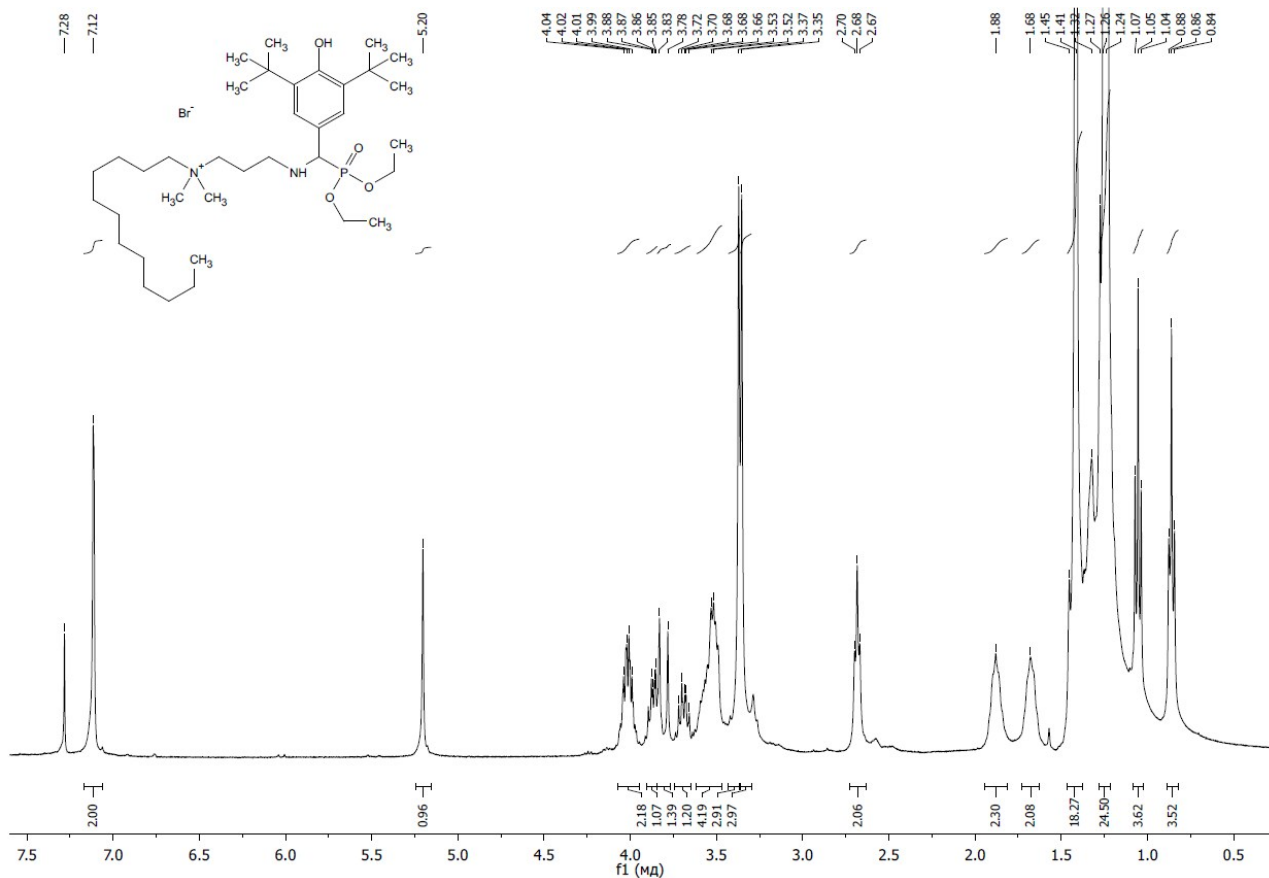


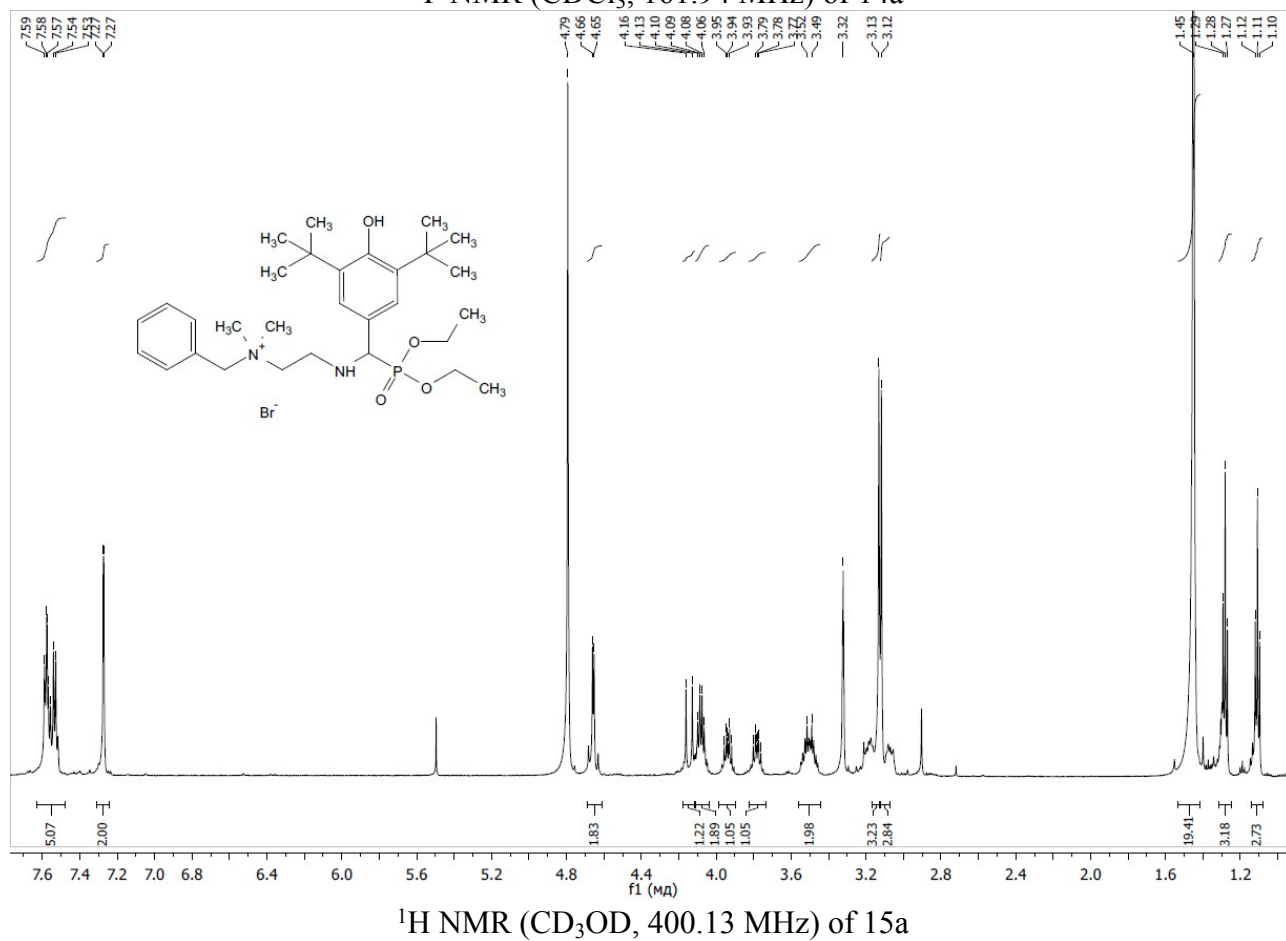
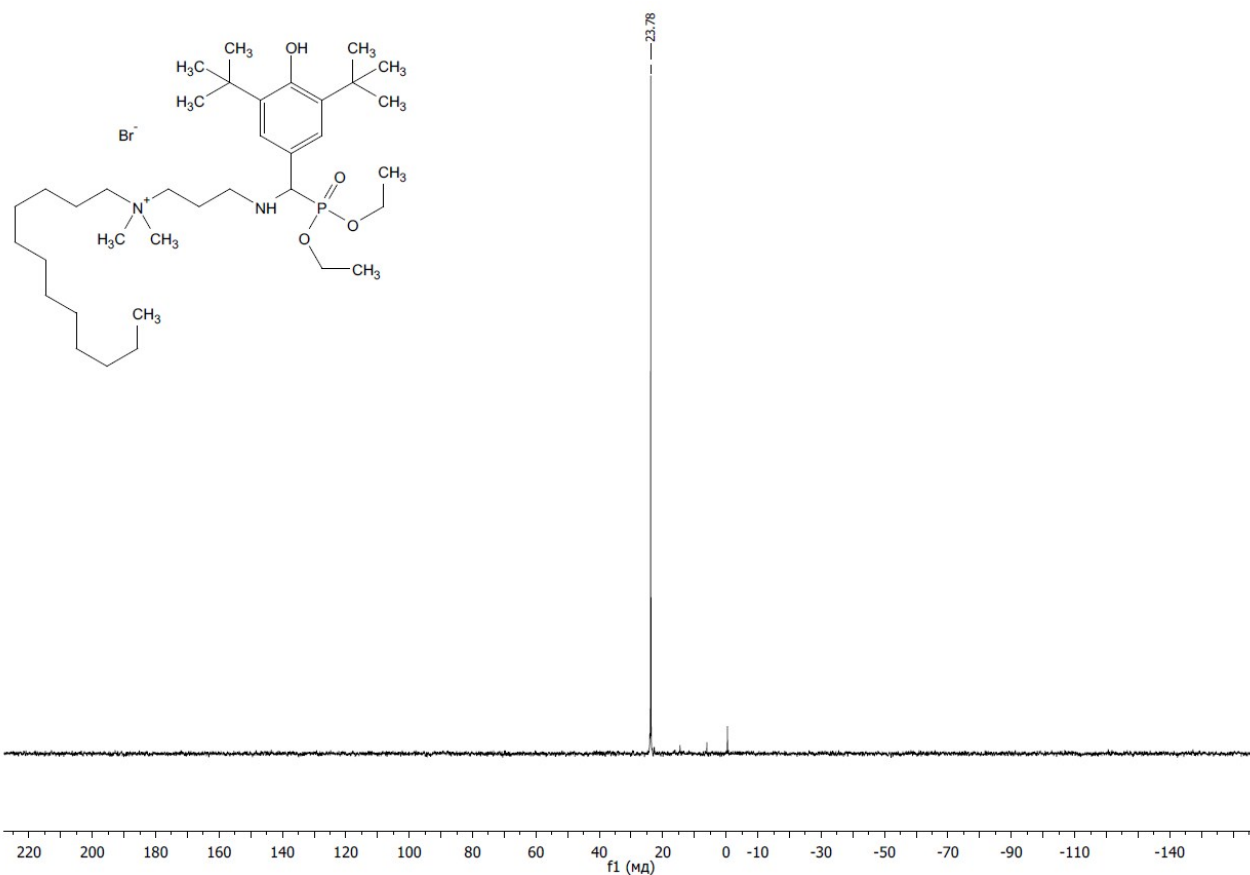


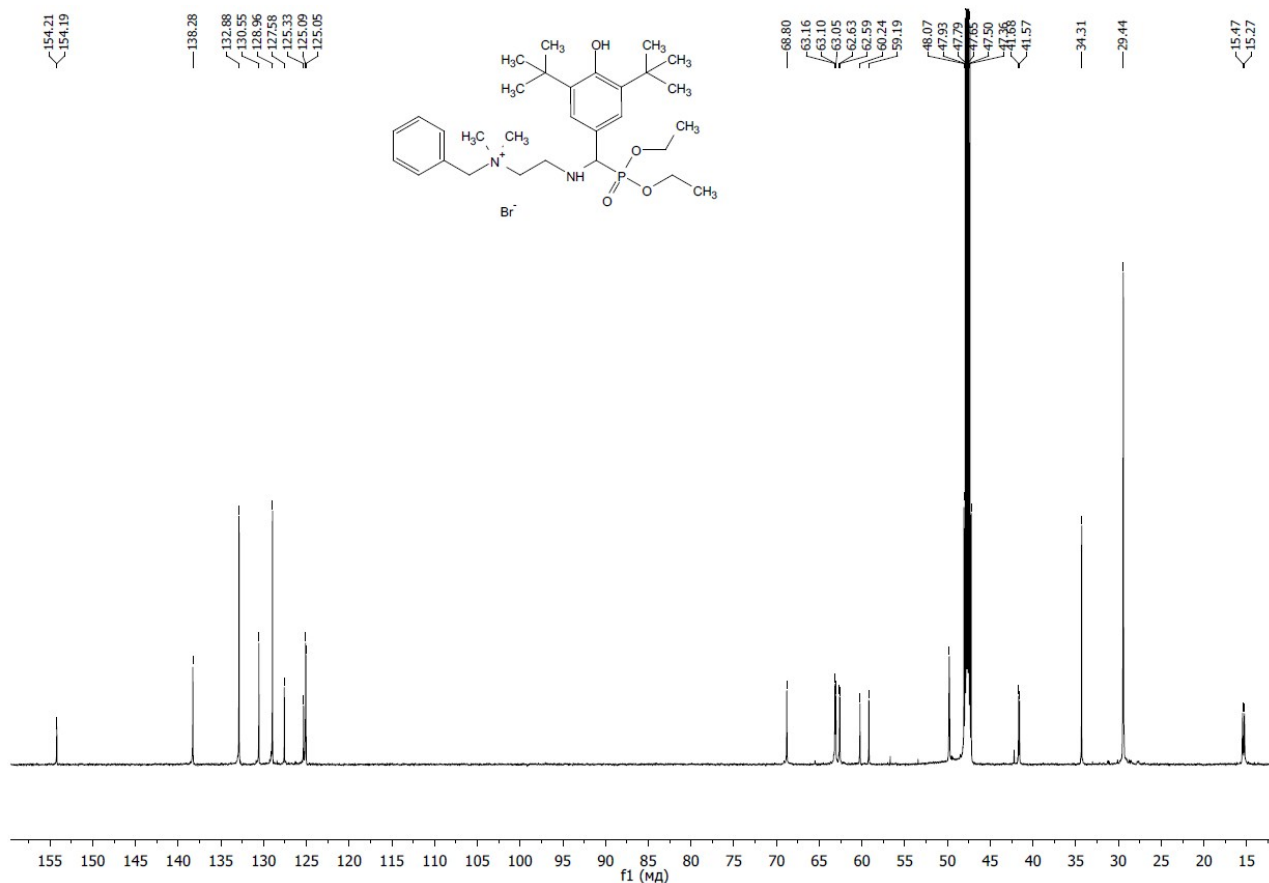




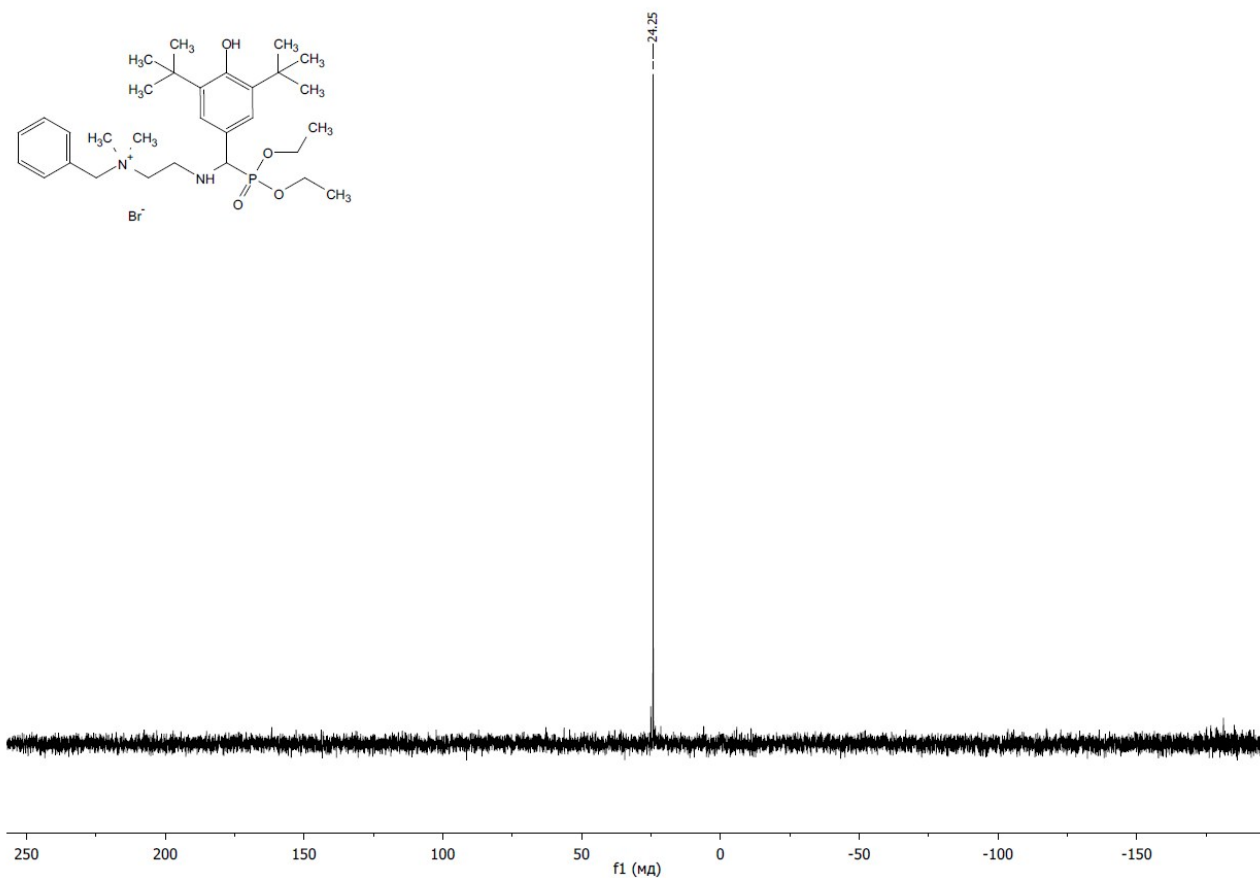




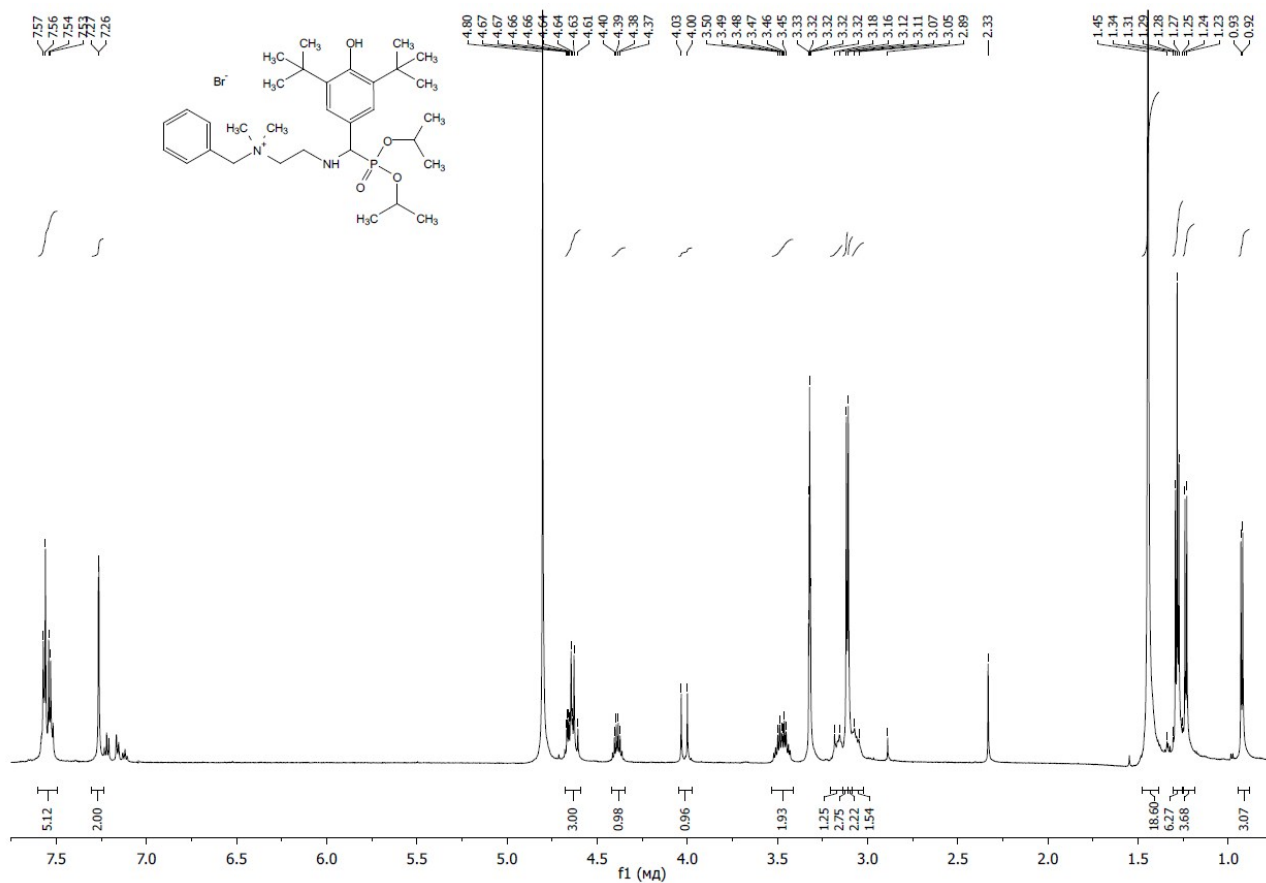




<sup>13</sup>C NMR (CD<sub>3</sub>OD, 150 MHz) of 15a



<sup>31</sup>P NMR (CD<sub>3</sub>OD, 161.94 MHz) of 15a



**<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400.13 MHz) of 15b**



**<sup>31</sup>P NMR (CDCl<sub>3</sub>, 161.94 MHz) of 15b**

