

## SUPPLEMENTARY FILE

# Synthesis of the First 2-Hydroxyanthraquinone Substituted Cyclotriphosphazenes and Their Cytotoxic Properties

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# COMPOUND 6

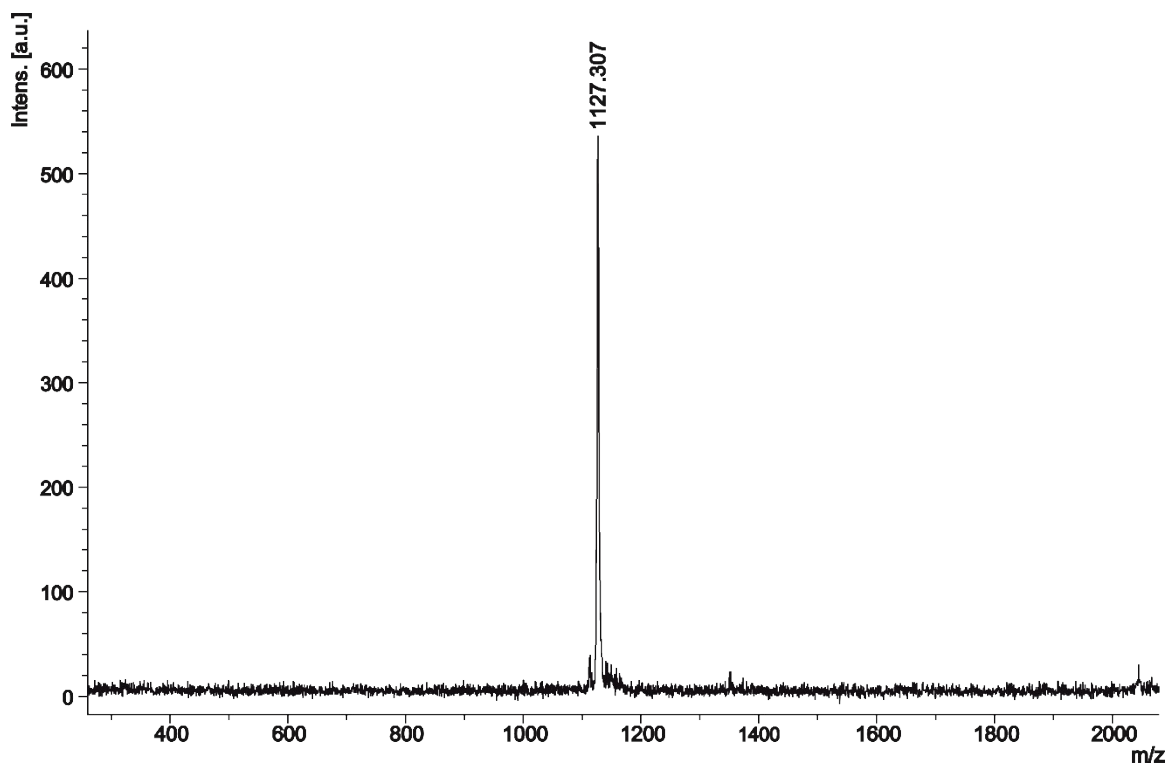


Figure S1. MALDI-MS spectra of Compound 6

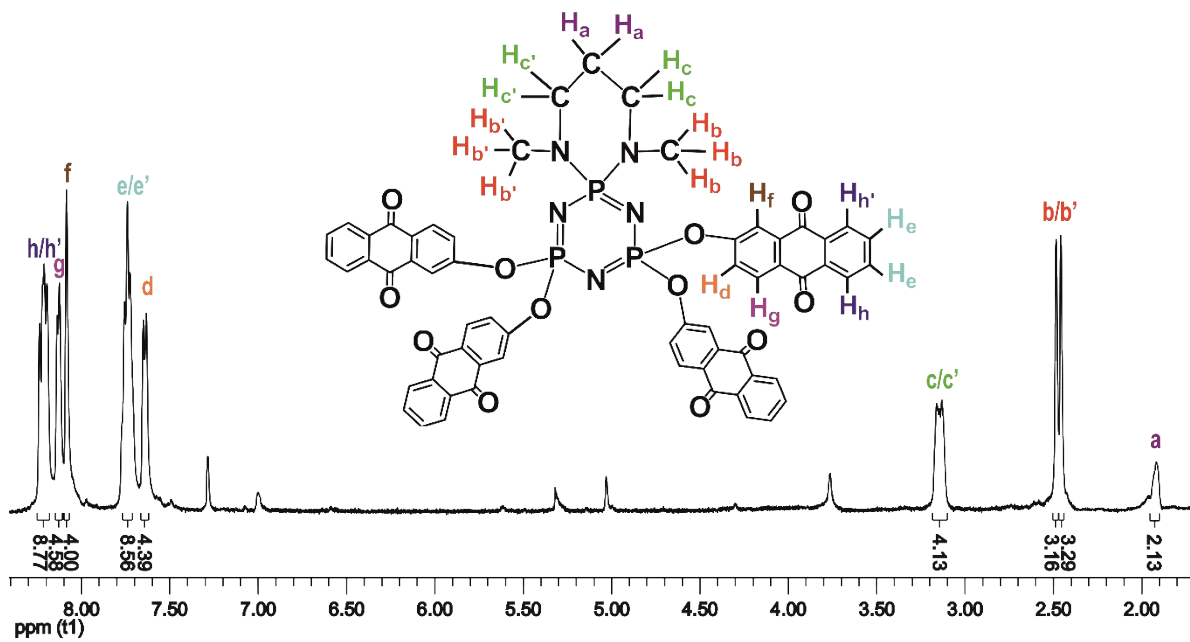


Figure S2. <sup>1</sup>H NMR spectra of Compound 6 in CDCl<sub>3</sub>

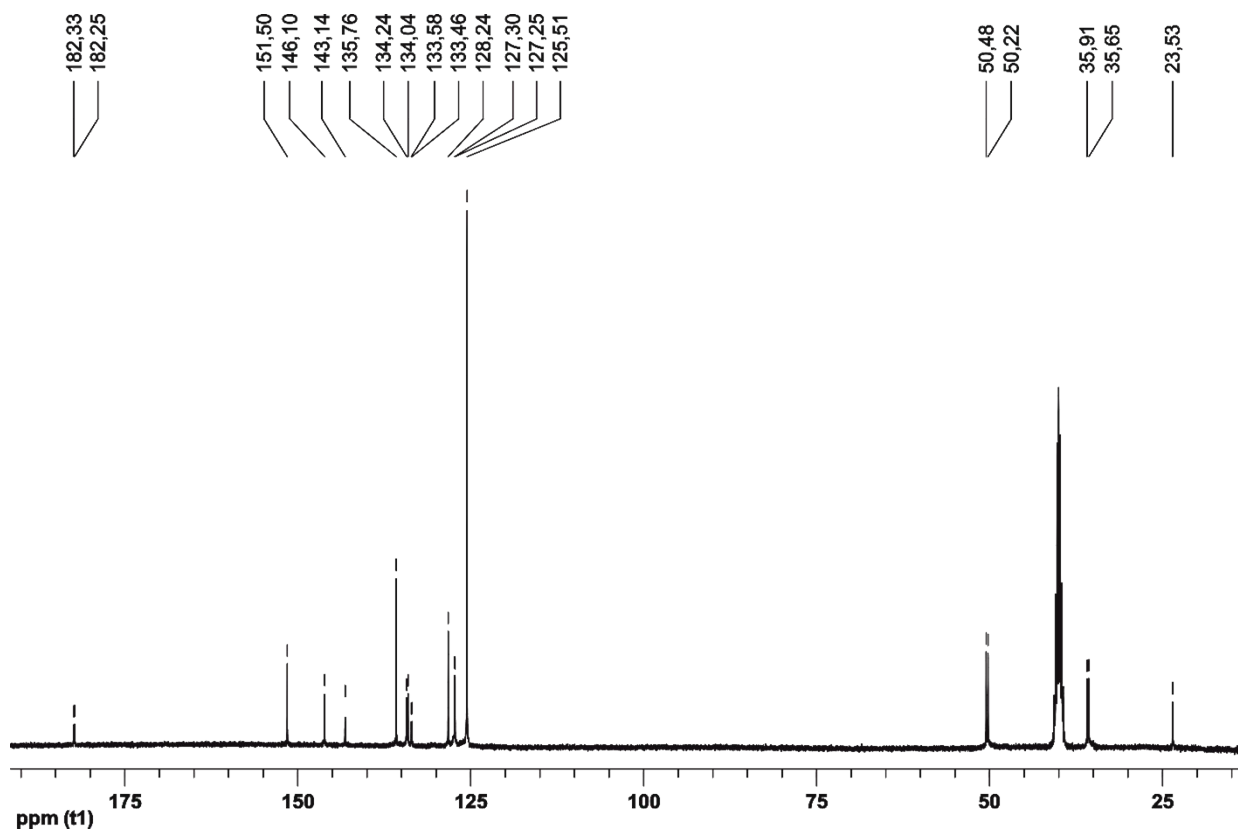


Figure S3.  $^{13}\text{C}$  NMR spectra of Compound 6 in  $\text{DMSO-d}_6$

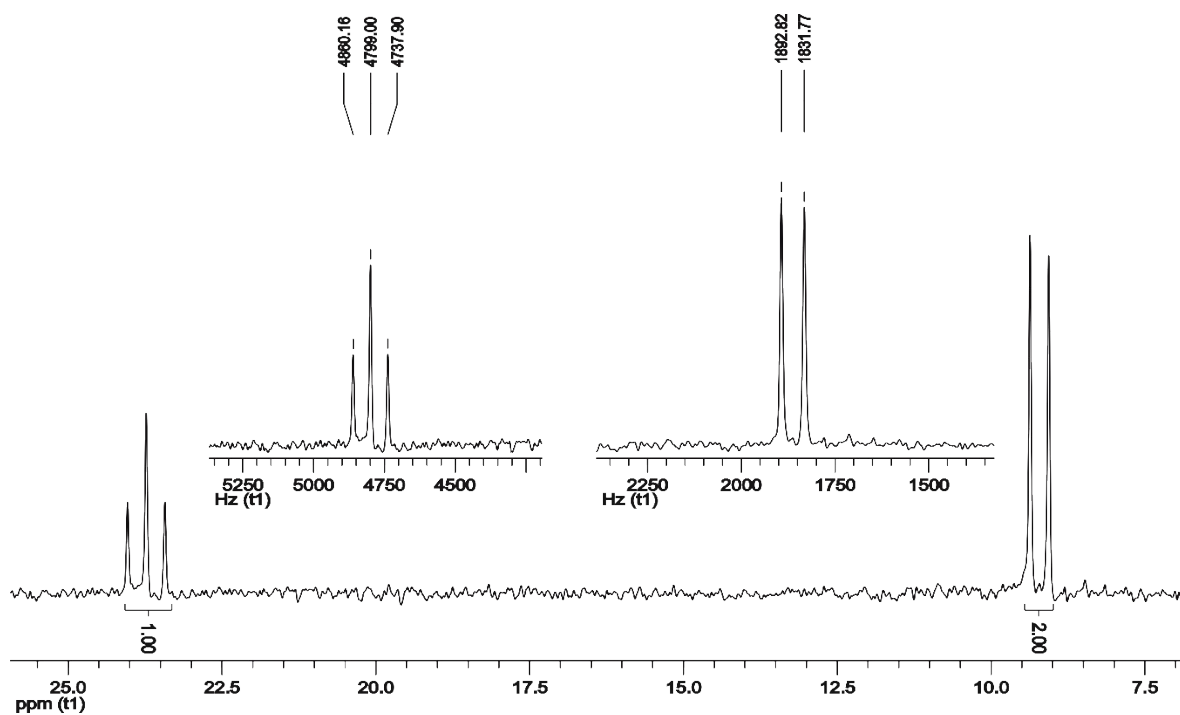
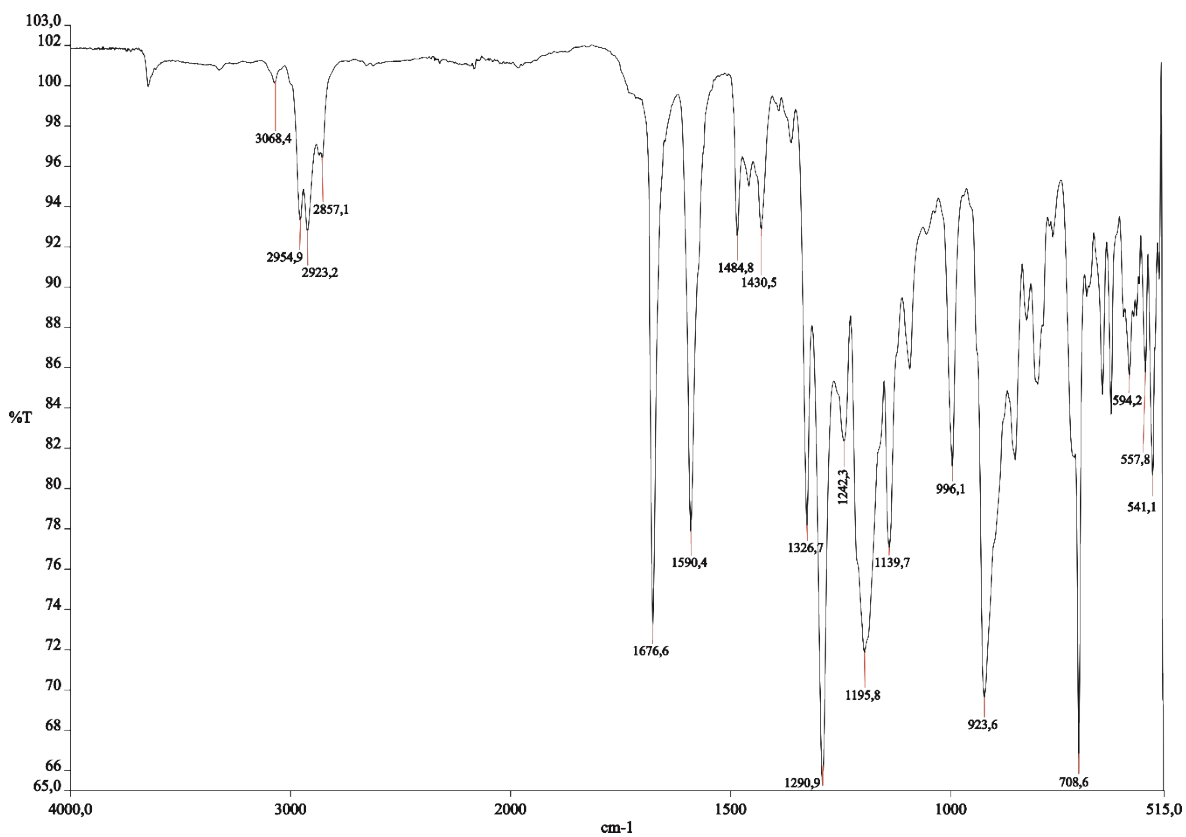


Figure S4.  $^{31}\text{P}$  NMR decoupled spectra of Compound 6 in  $\text{CDCl}_3$



**Figure S5.** FT-IR spectra of Compound 6

# COMPOUND 7

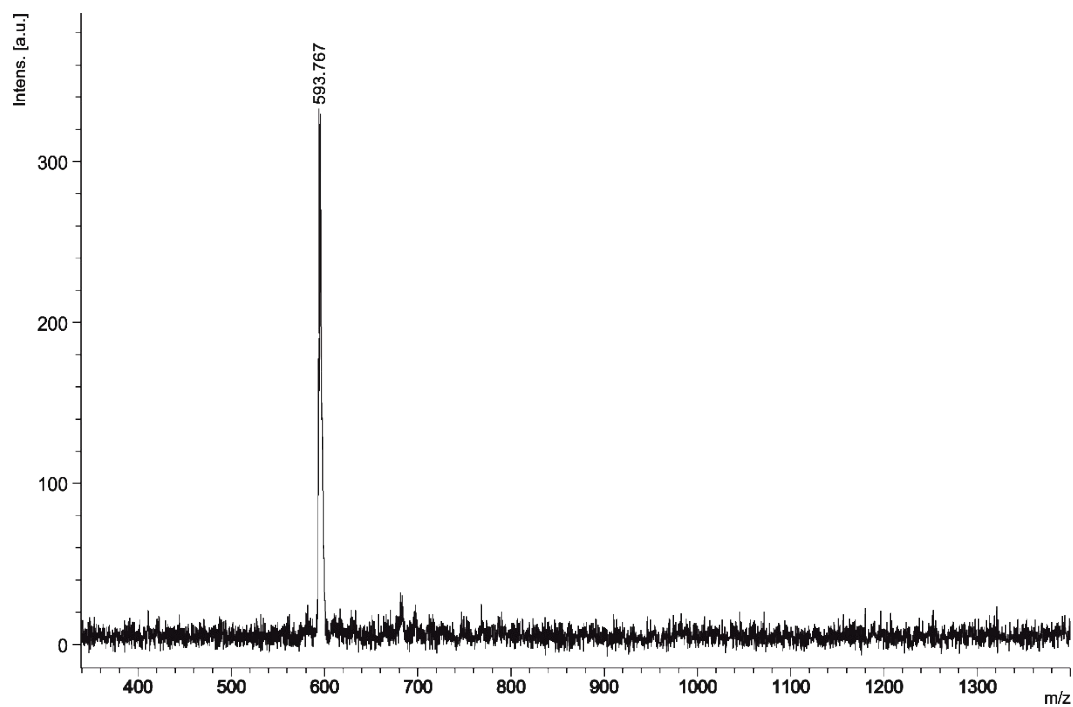


Figure S6. MALDI-MS spectra of Compound 7

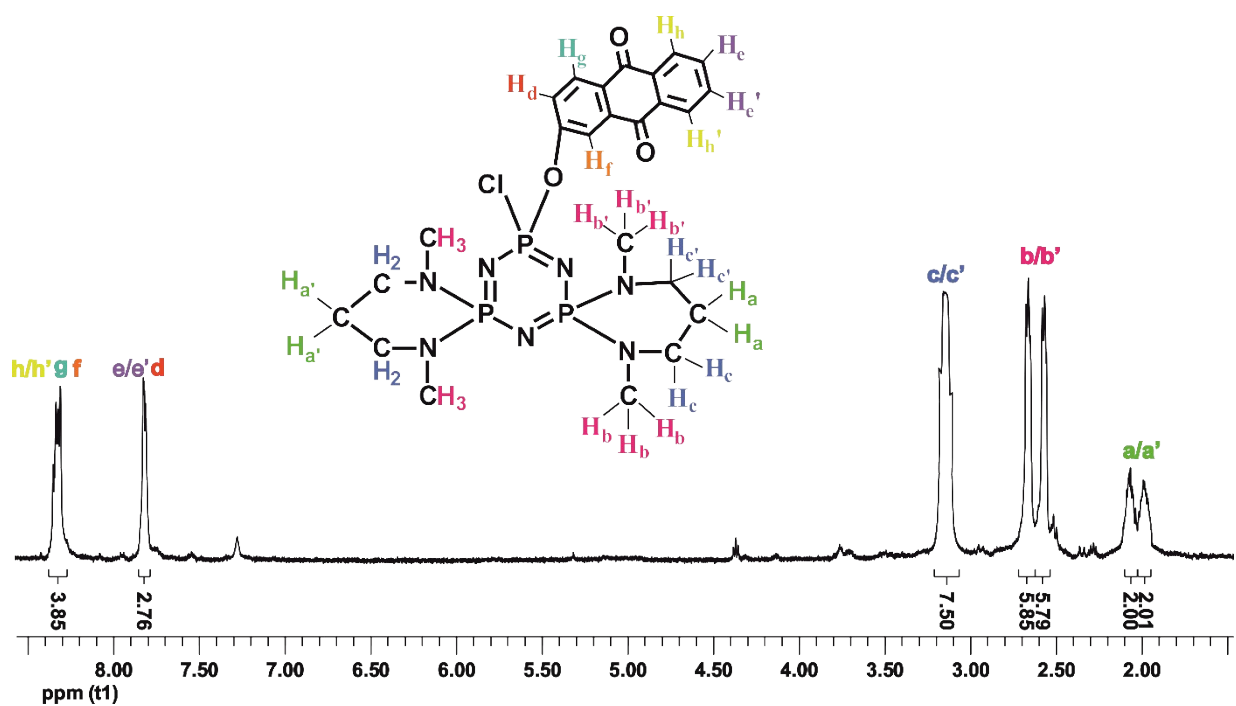
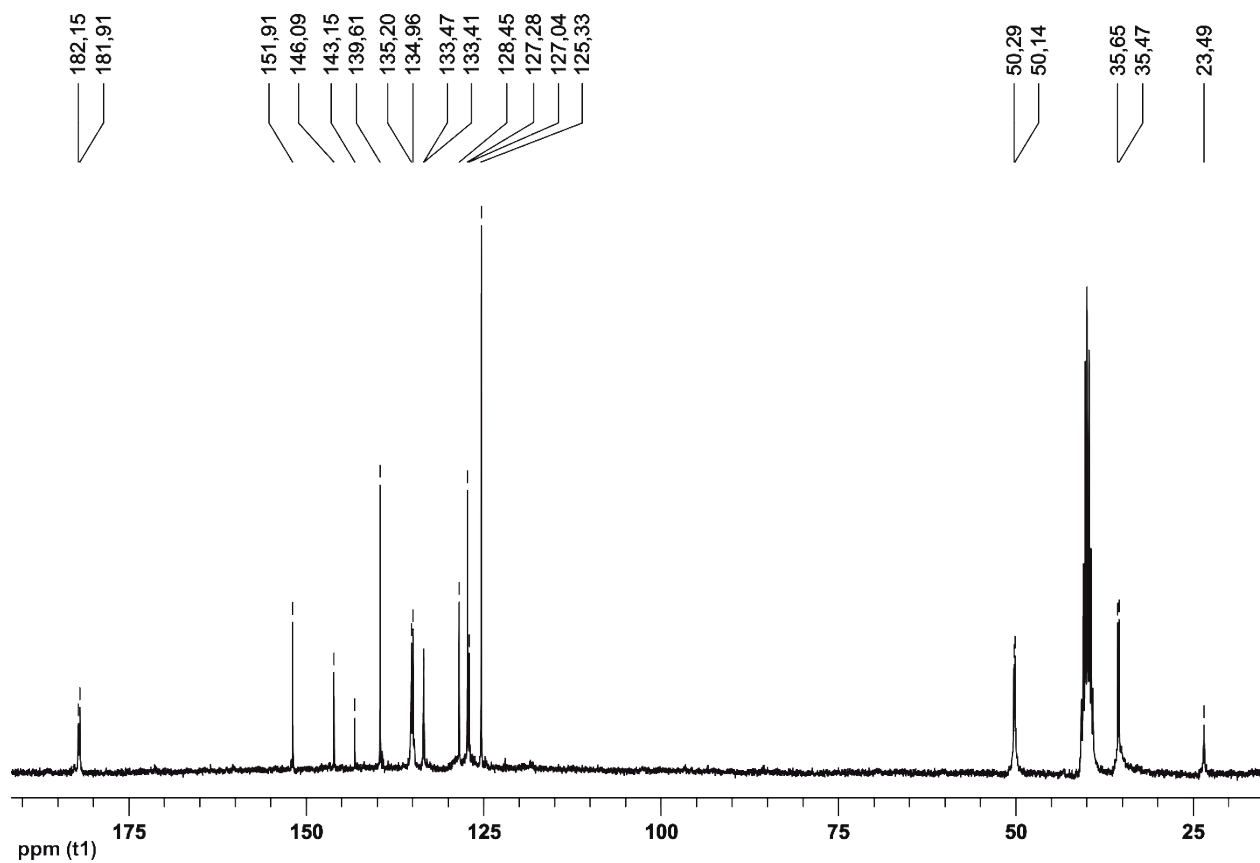
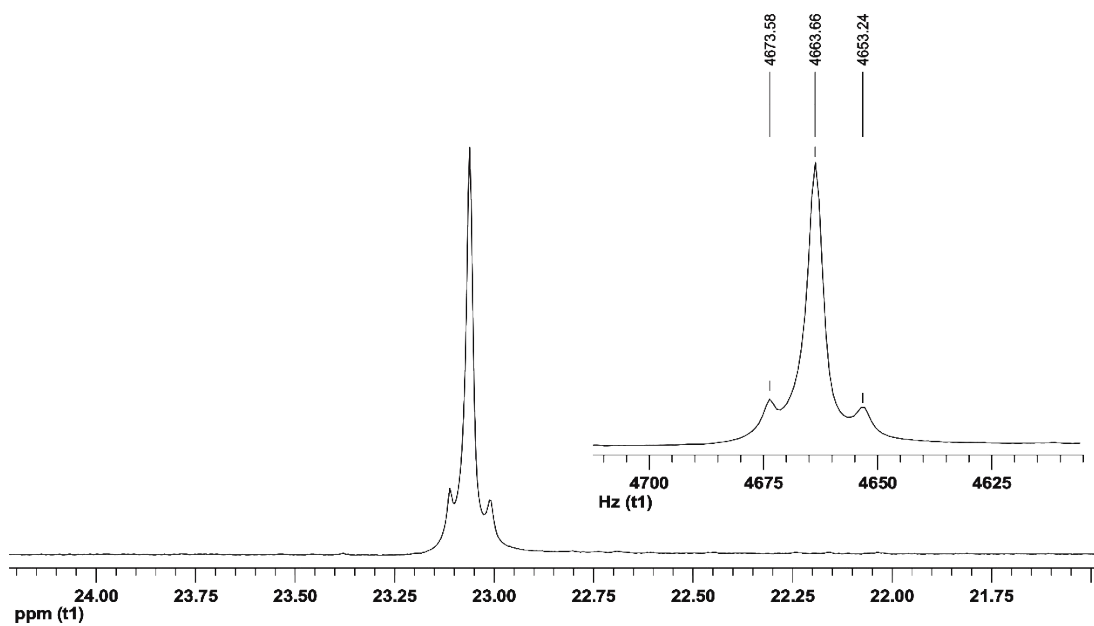


Figure S7. <sup>1</sup>H NMR spectra of Compound 7 in CDCl<sub>3</sub>



**Figure S8.**  $^{13}\text{C}$  NMR spectra of Compound 7 in  $\text{DMSO-d}_6$



**Figure S9.**  $^{31}\text{P}$  NMR decoupled spectra of Compound 7 in  $\text{CDCl}_3$



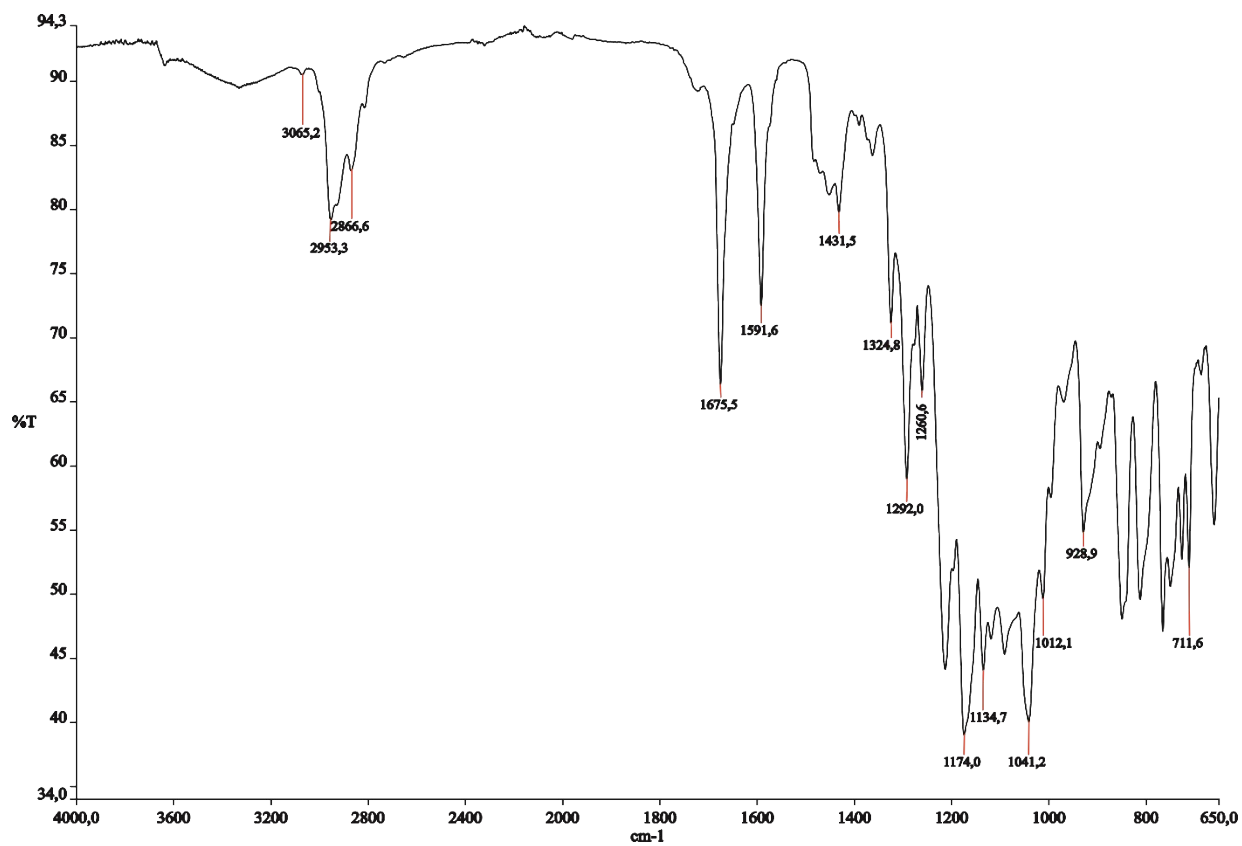


Figure S10. FT-IR spectra of Compound 7

## COMPOUND 8

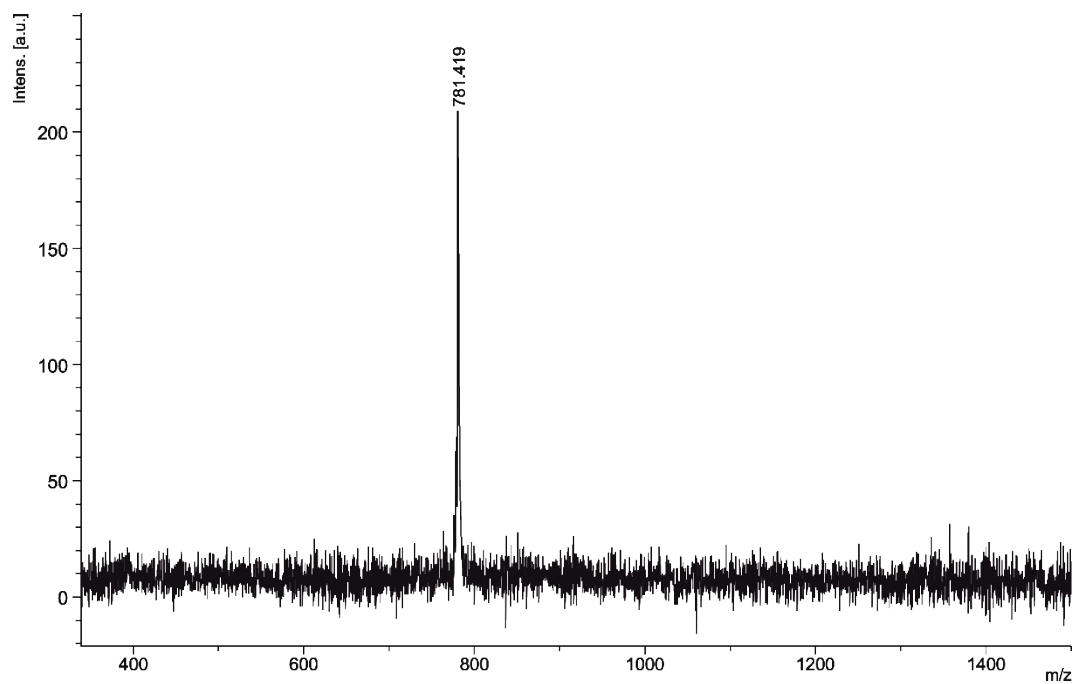


Figure S11. MALDI-MS spectra of Compound 8

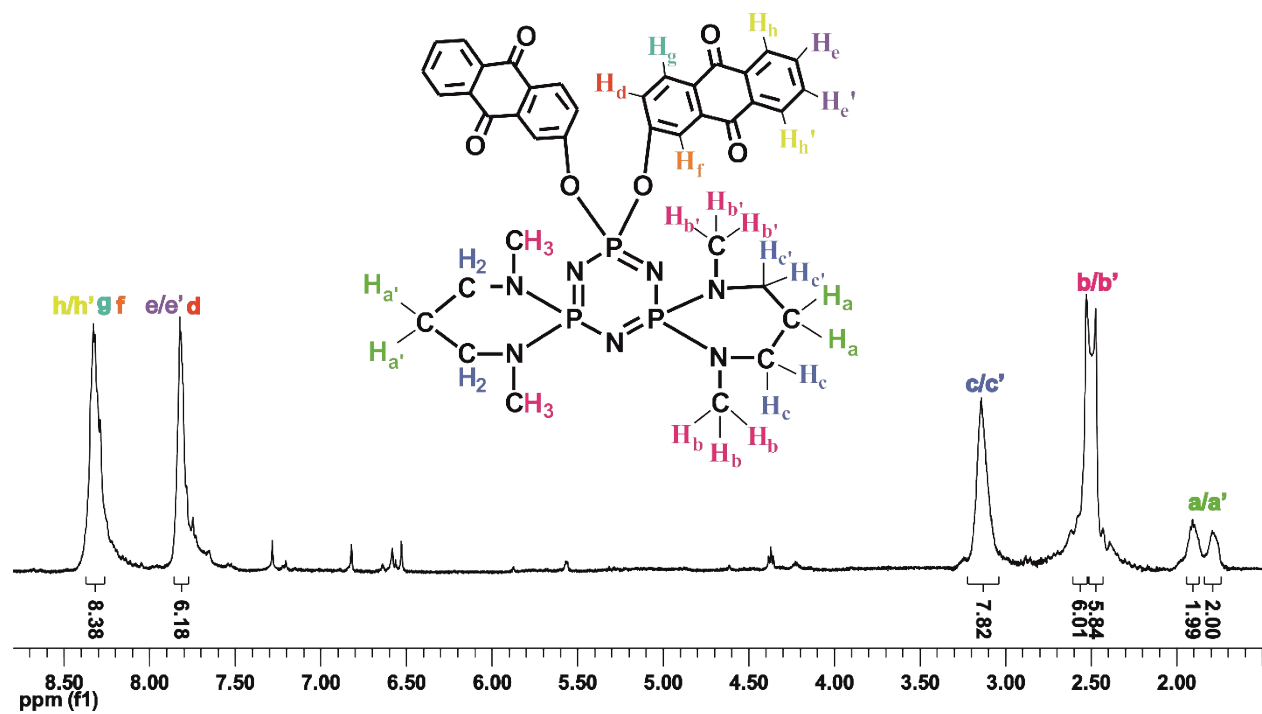


Figure S12. <sup>1</sup>H NMR spectra of Compound 8 in CDCl<sub>3</sub>

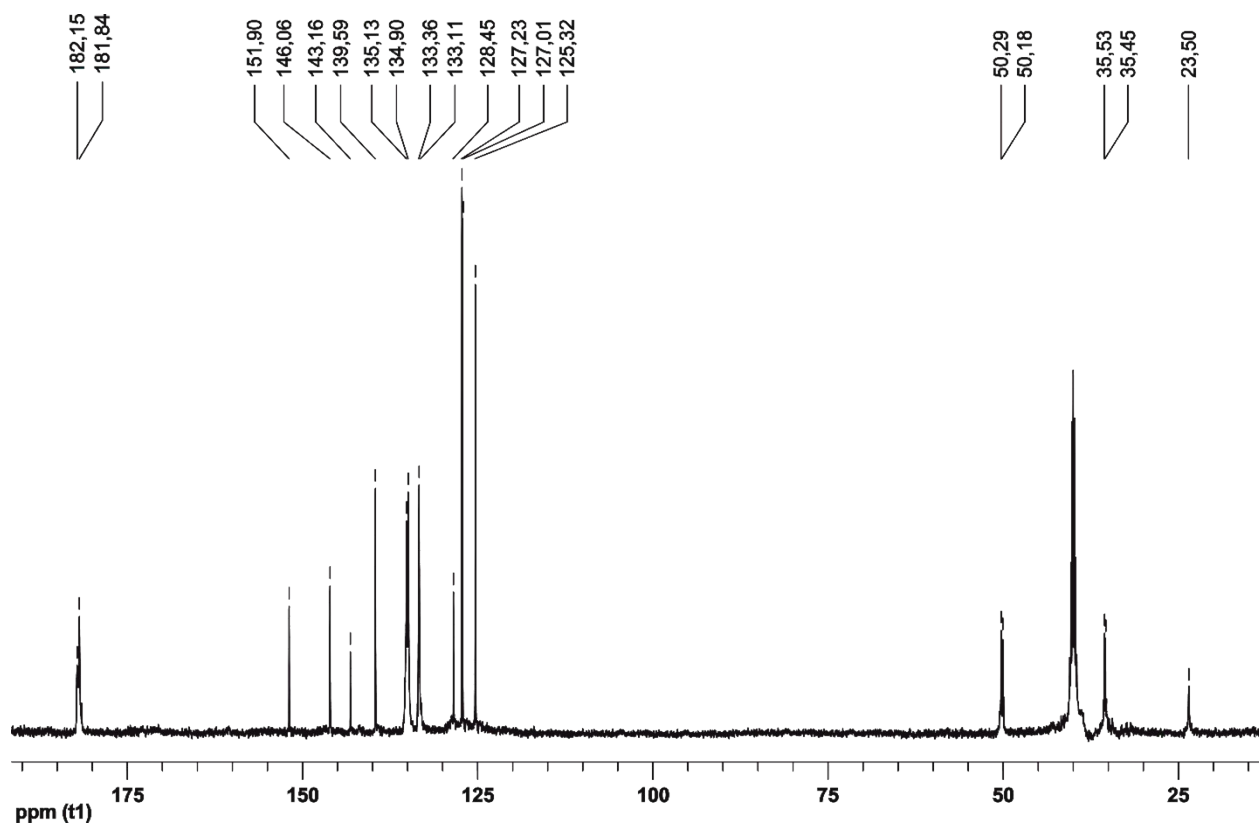


Figure S13.  $^{13}\text{C}$  NMR spectra of Compound 8 in  $\text{DMSO-d}_6$

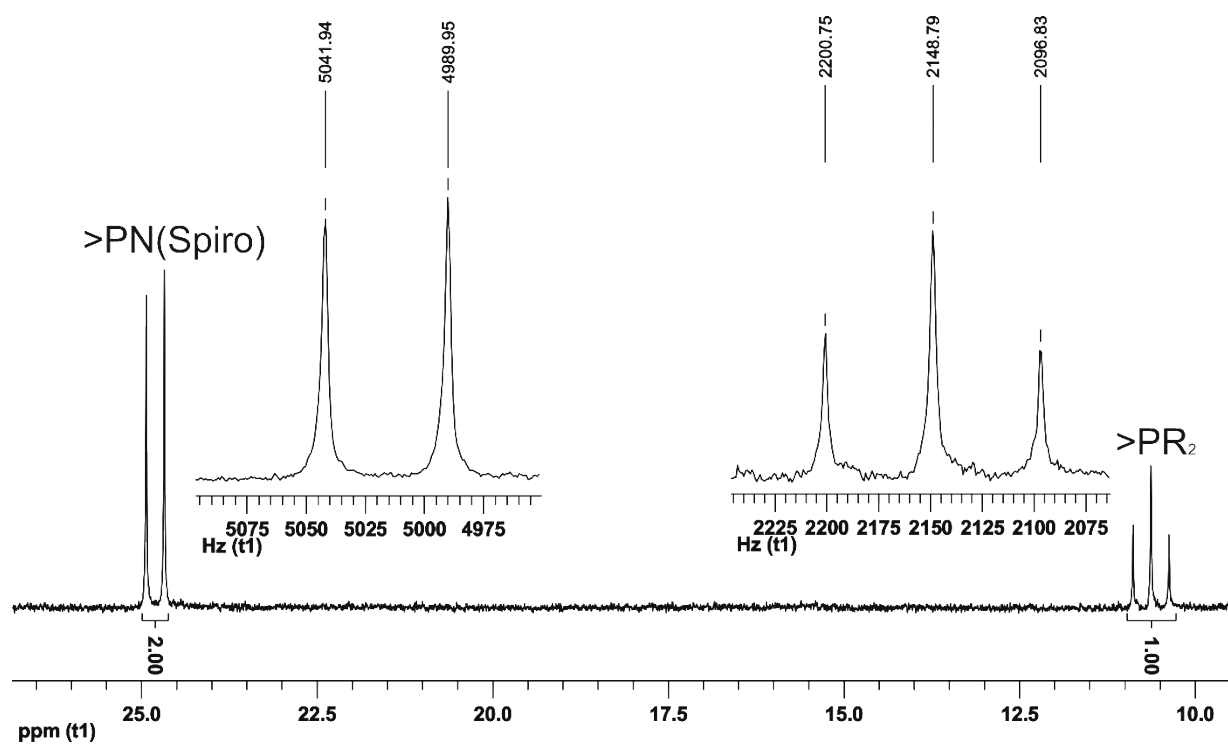


Figure S14.  $^{31}\text{P}$  NMR decoupled spectra of Compound 8 in  $\text{CDCl}_3$

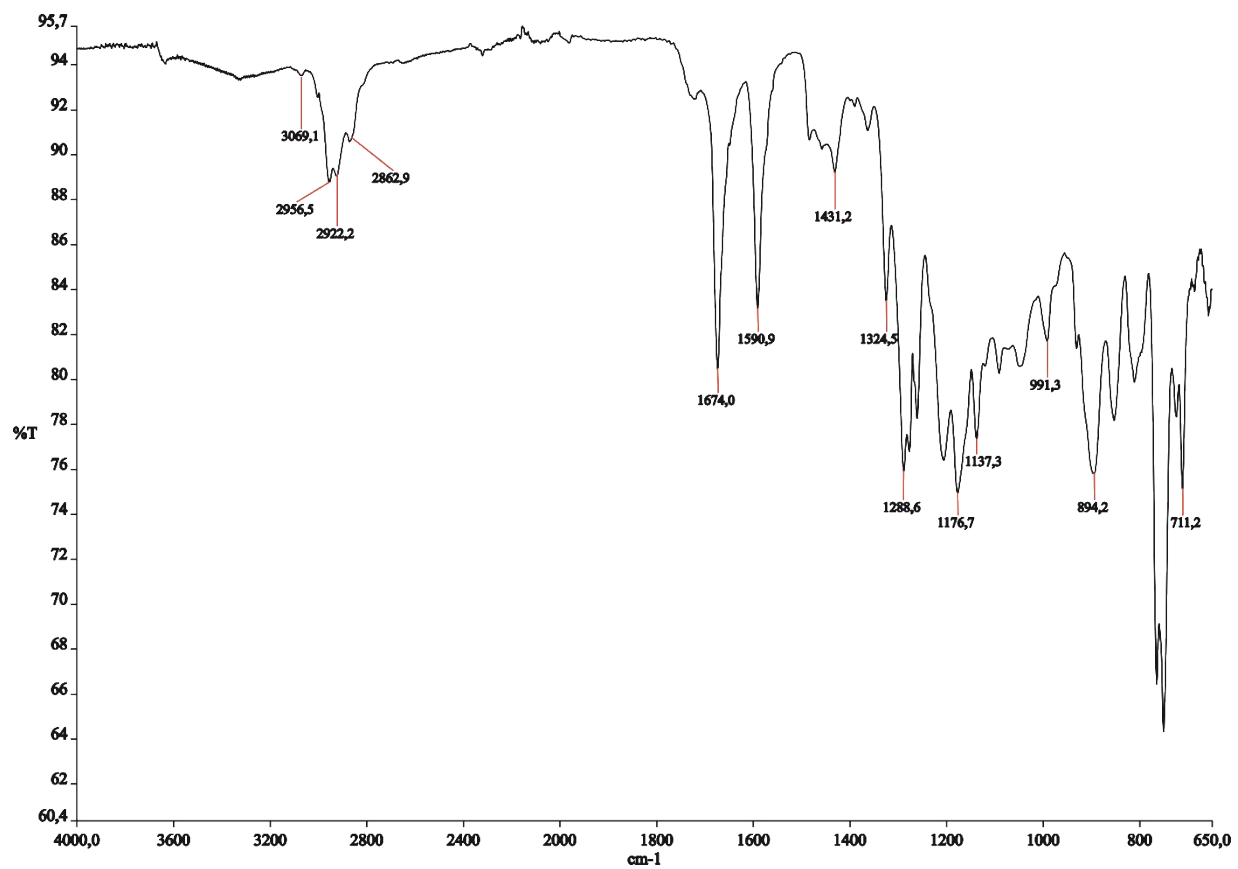


Figure S15. FT-IR spectra of Compound 8

## COMPOUND 9

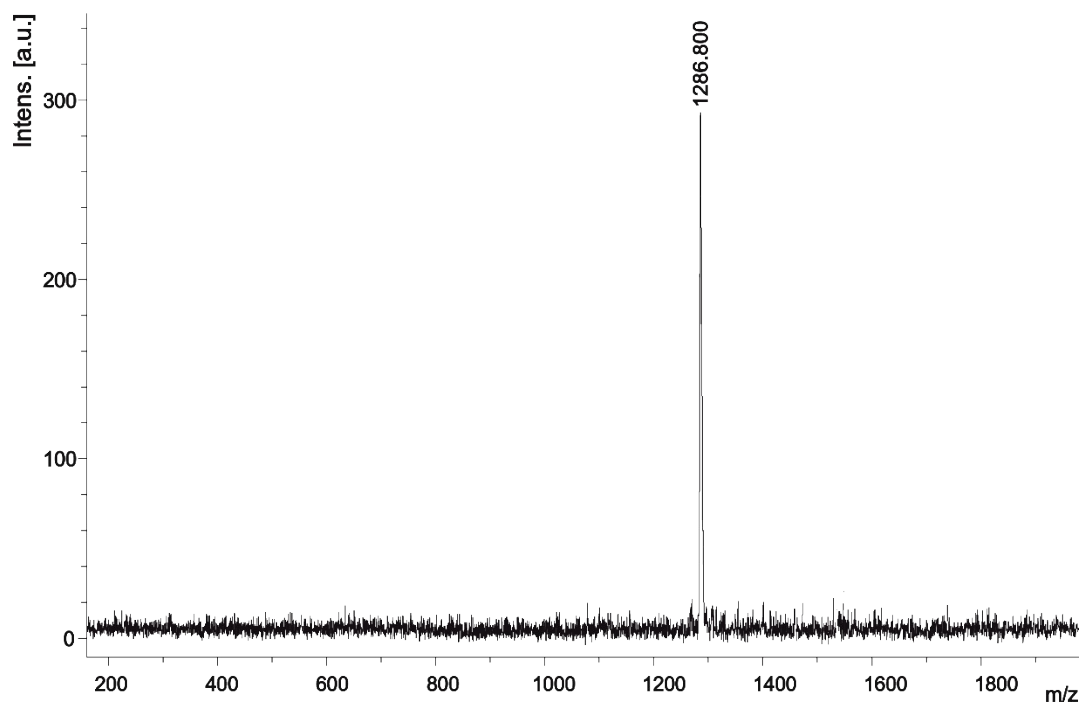


Figure S16. MALDI-MS spectra of Compound 9

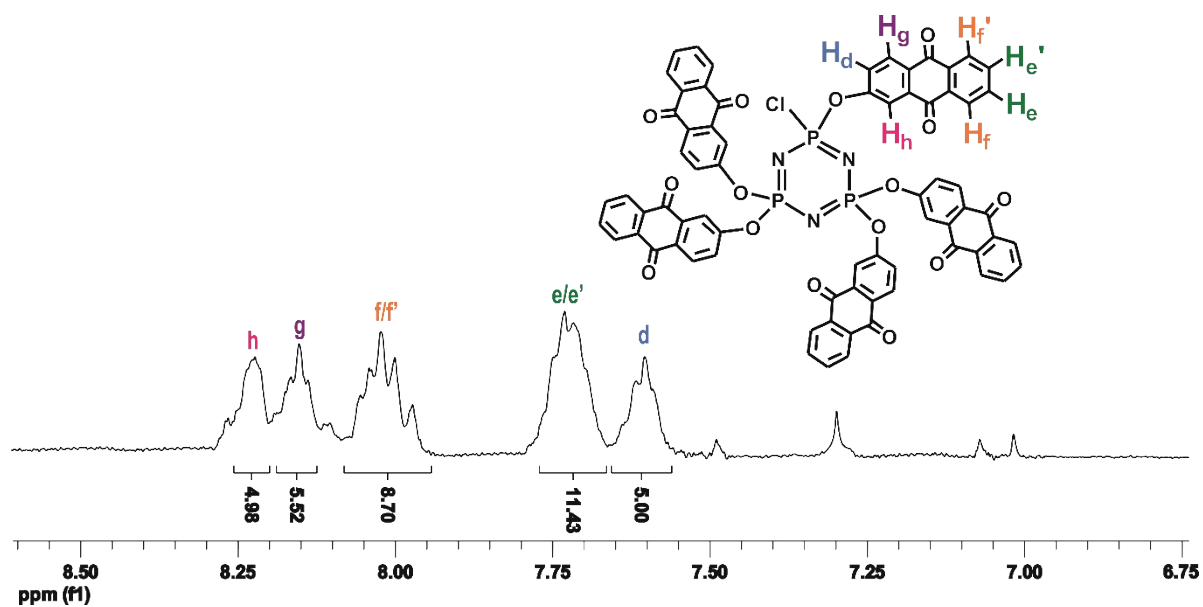


Figure S17. <sup>1</sup>H NMR spectra of Compound 9 in CDCl<sub>3</sub>

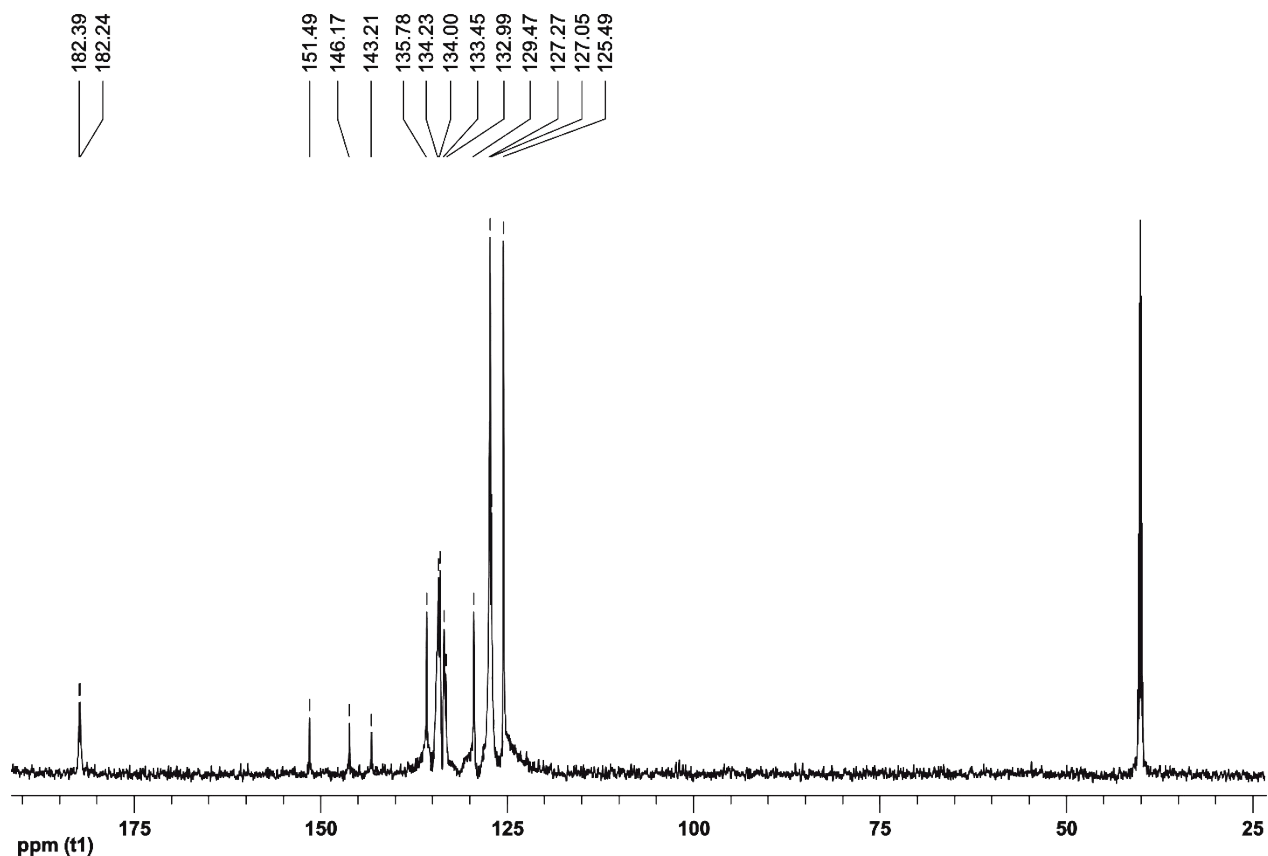
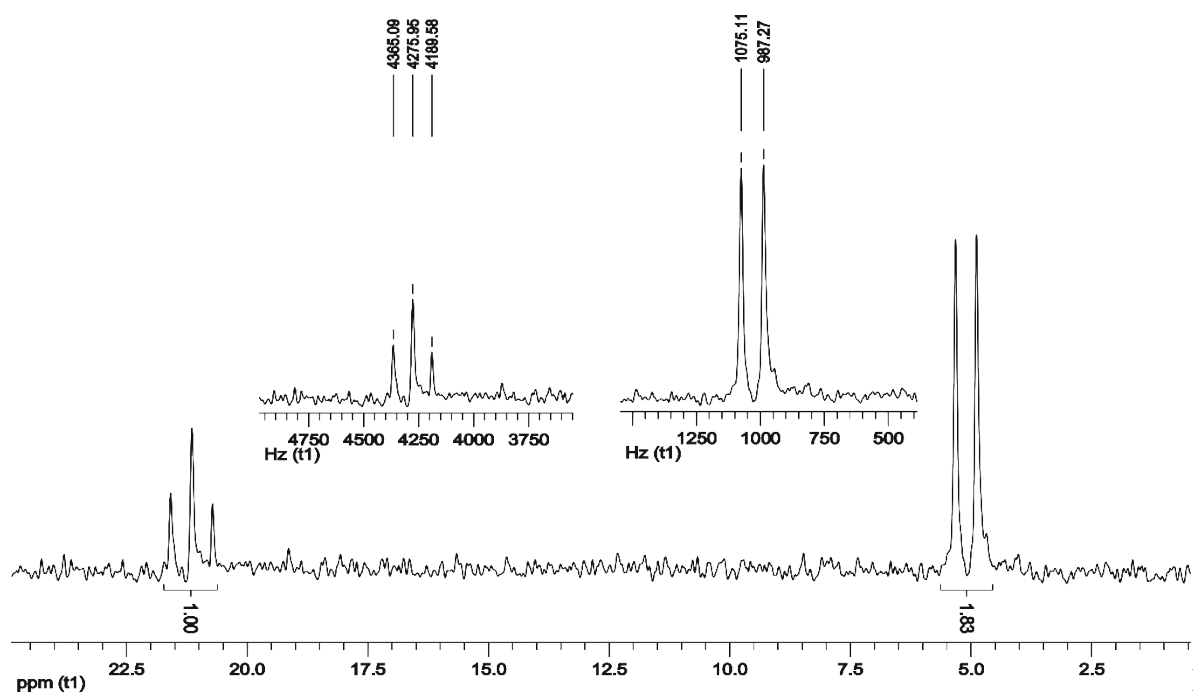
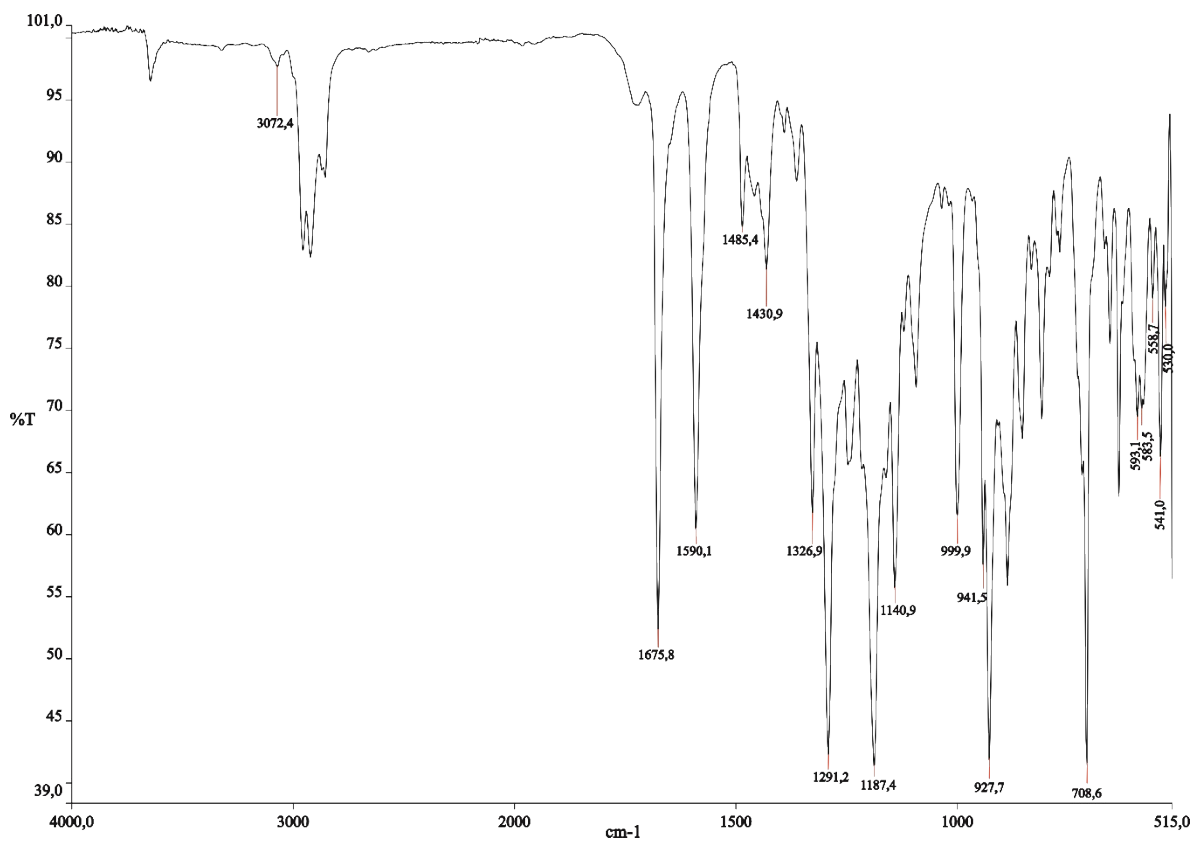


Figure S18.  $^{13}\text{C}$  NMR spectra of Compound 9 in  $\text{DMSO-d}_6$



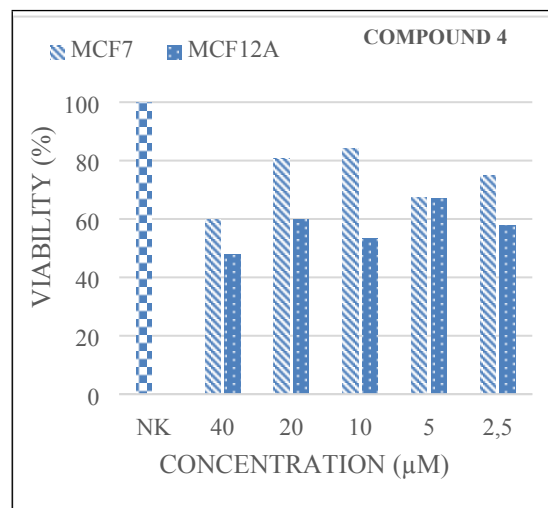
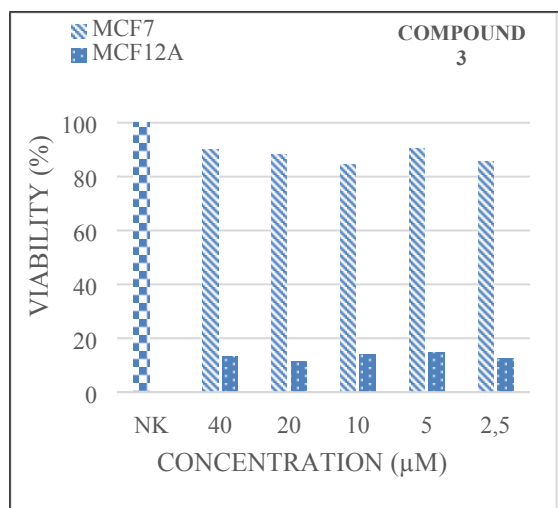
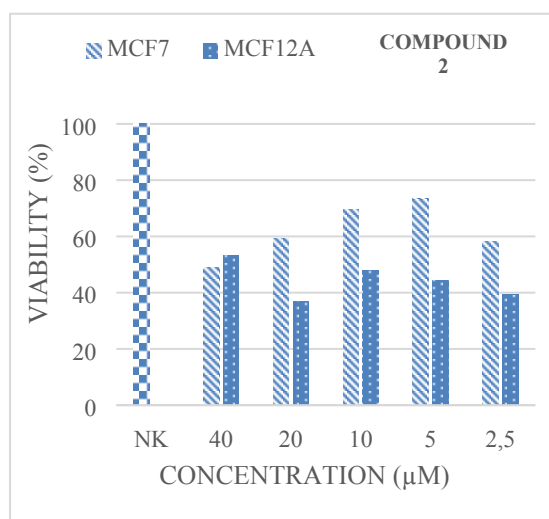
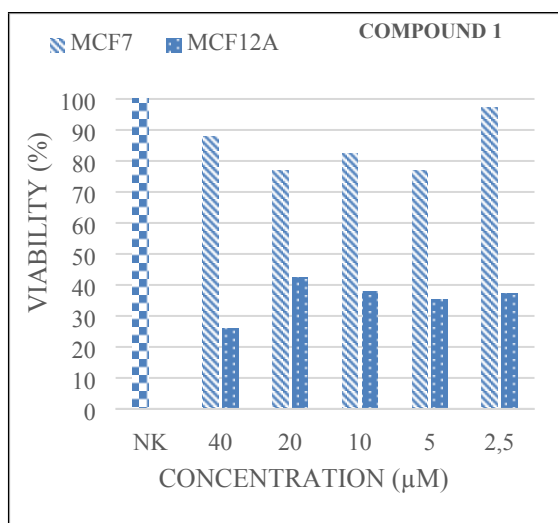
re S19.  $^{31}\text{P}$  NMR decoupled spectra of Compound 9 in  $\text{CDCl}_3$

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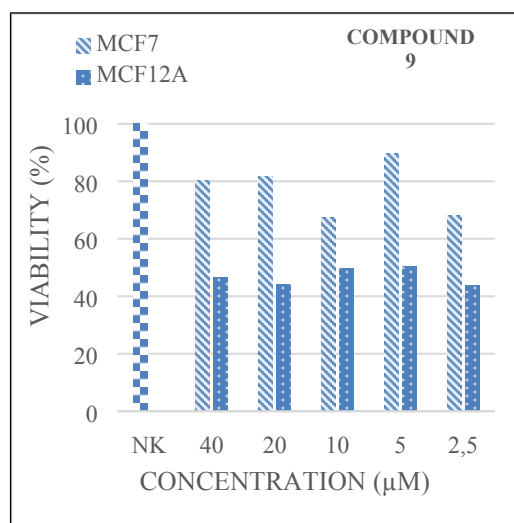
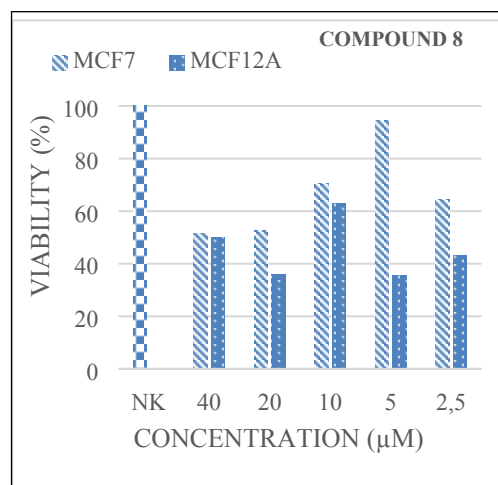
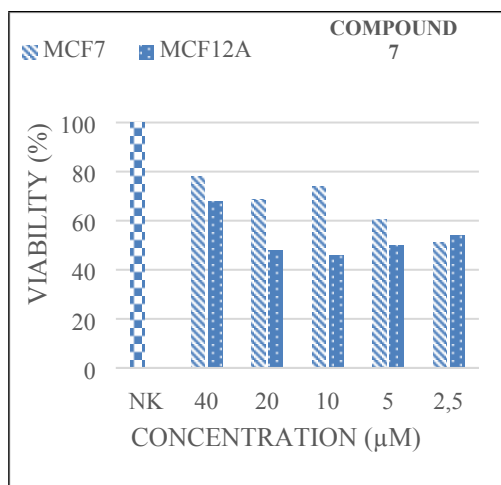
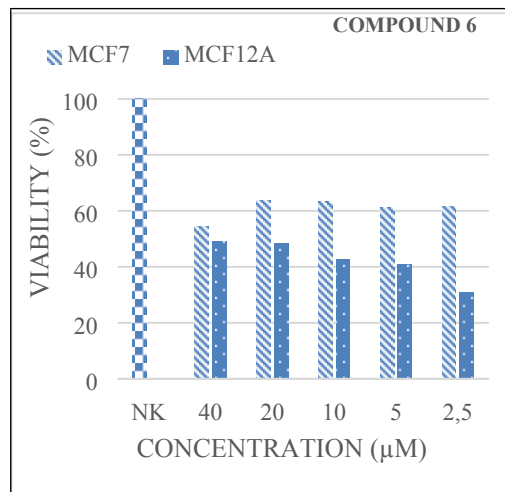
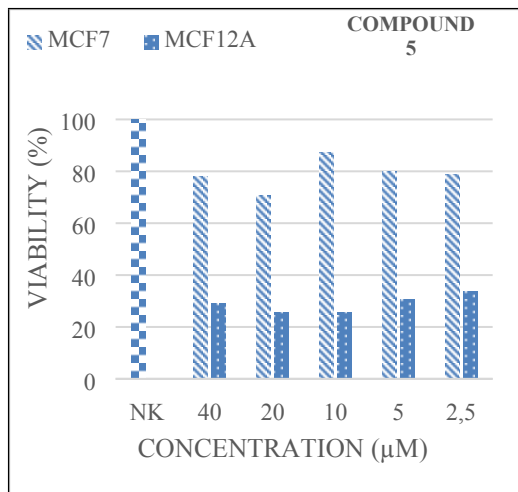


**Figure S20.** FT-IR spectra of Compound 9

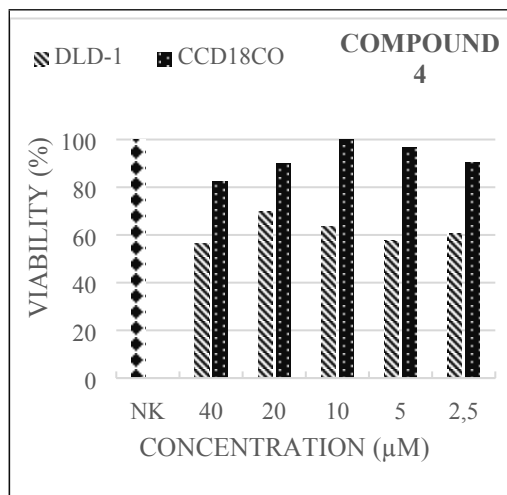
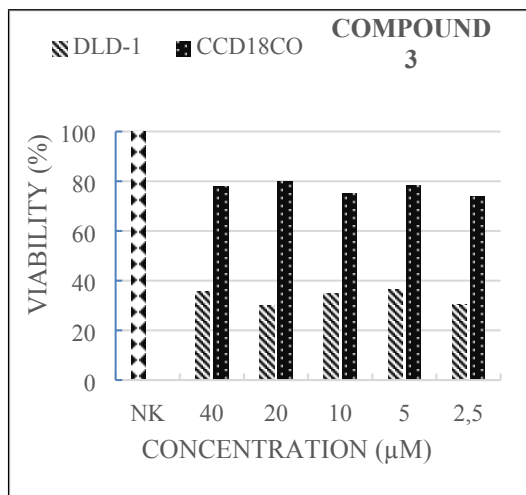
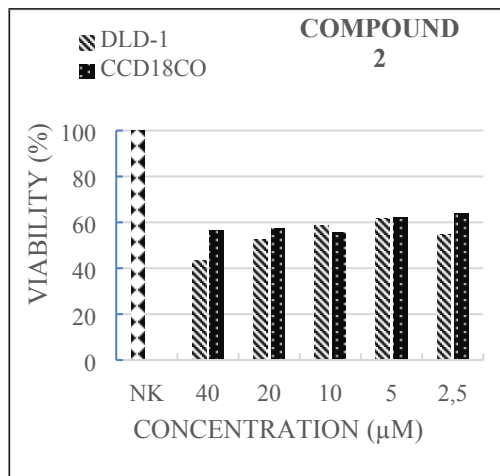
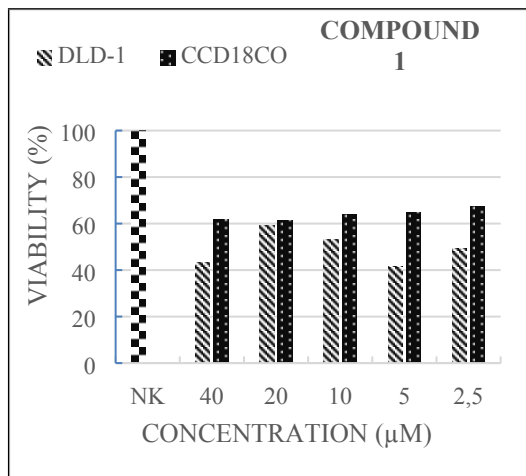
**Figure S21.** Graphics of the concentrations values of compounds applied in the MCF-7 and MCF12A cell lines according to viability (%) with MTT method.

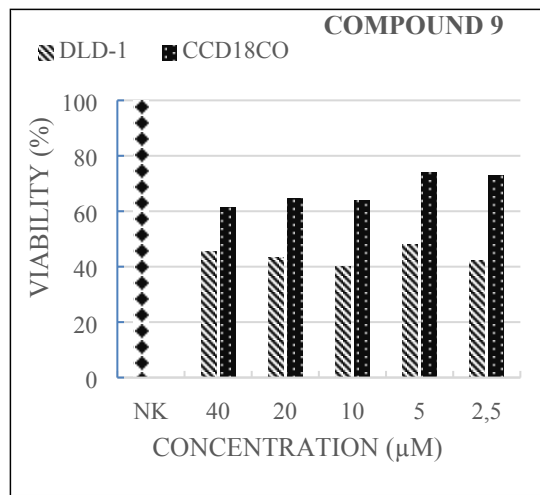
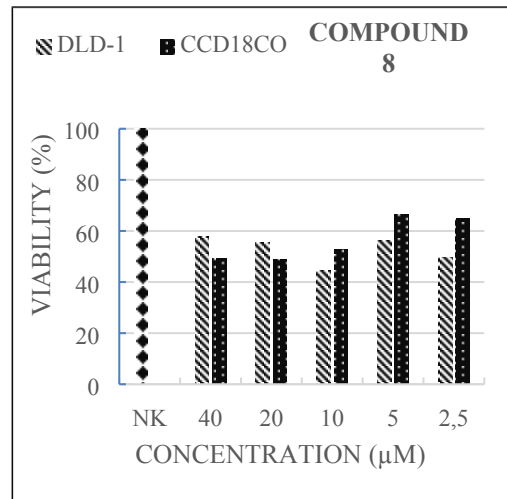
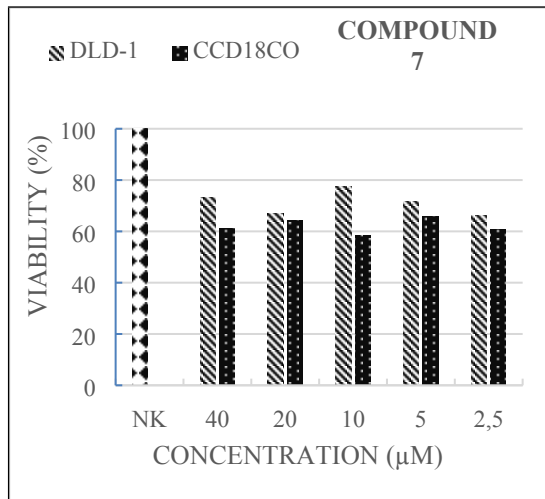
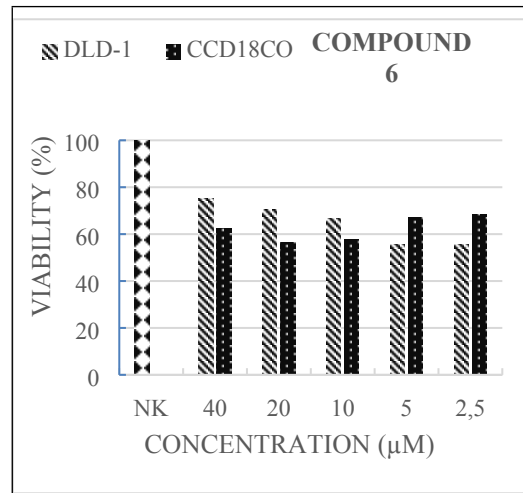
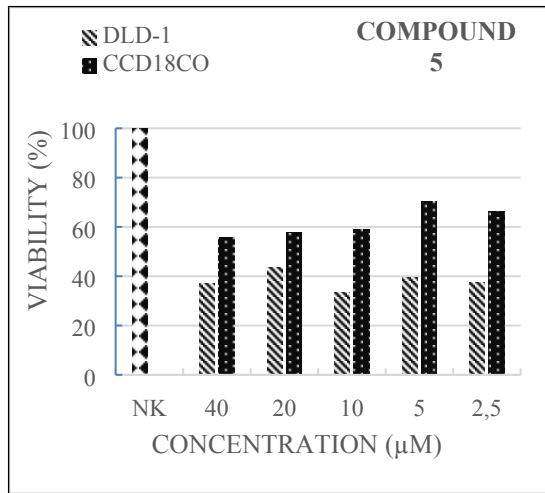






**Figure S22.** MTT analysis results of compounds in cells. Graphics of the concentrations of compounds applied in the DLD1 and CCD-18CO cell lines according to absorbance with MTT method





**Table S1.** Selectivity of the cytotoxicity of anthraquinone derivatives compounds to two cancer cells as compared with normal cells.

Compound No	IC <sub>50</sub> (μM) <sup>a</sup>			
	MCF-7	MCF-12A	DLD-1	CCD-18Co
1	20	20	40	20
2	40	40	20	10
3	10	5	40	2.5
4	40	10	5	40
5	20	2.5	20	40
6	40	40	5	20
7	2.5	40	40	10
8	40	10	2.5	40
9	10	5	10	40

<sup>a</sup>The selectivity index is the ratio of the IC<sub>50</sub> values of the treatments on normal cells to those in the cancer cell lines.