

## Multicomponent Molecular Systems Based on Porphyrins, 1,3,5-Triazine and Carboranes: Synthesis and Characterization

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1. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4,6-bis(*m*-carborane-9'-yl)thio]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrin (5)

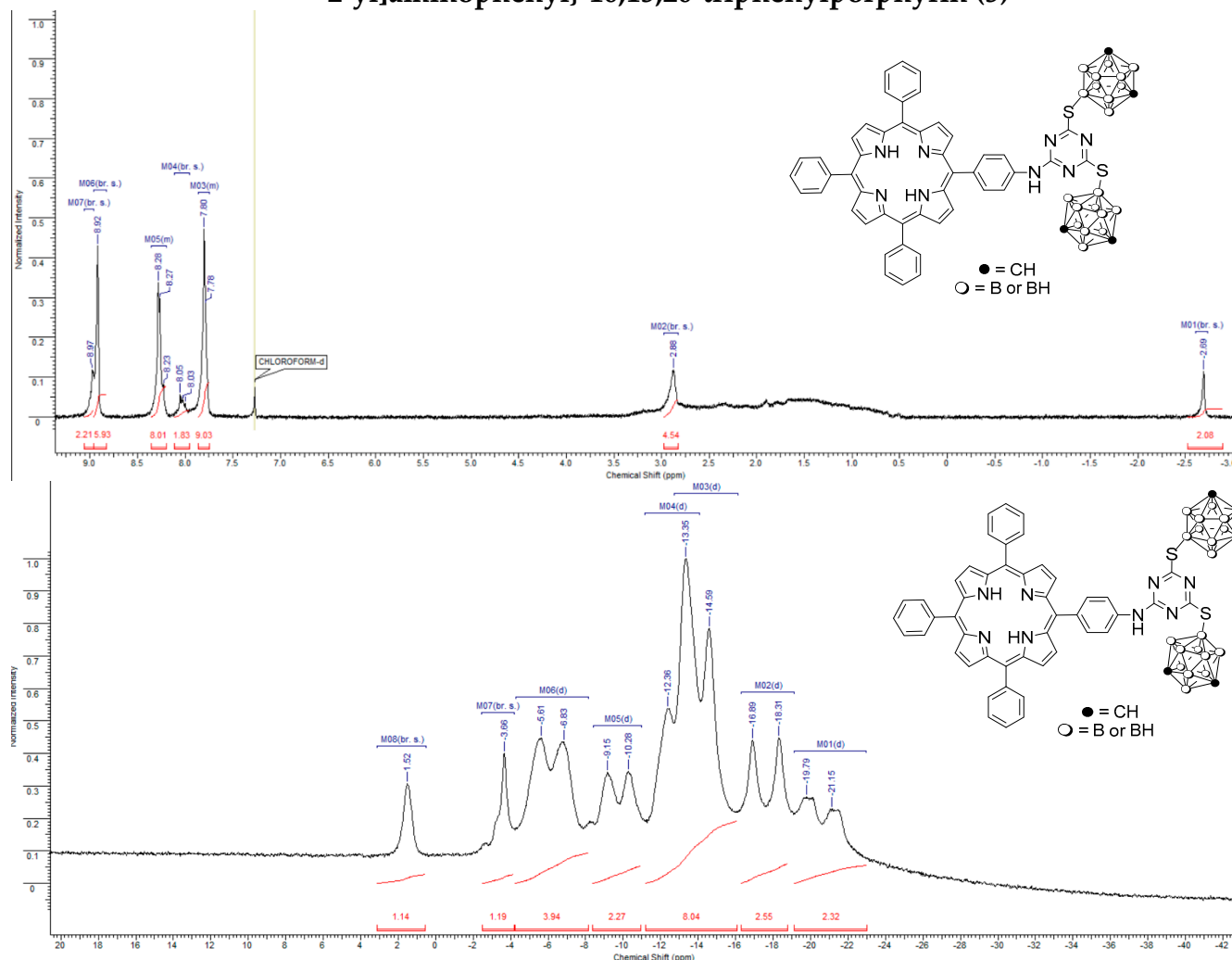
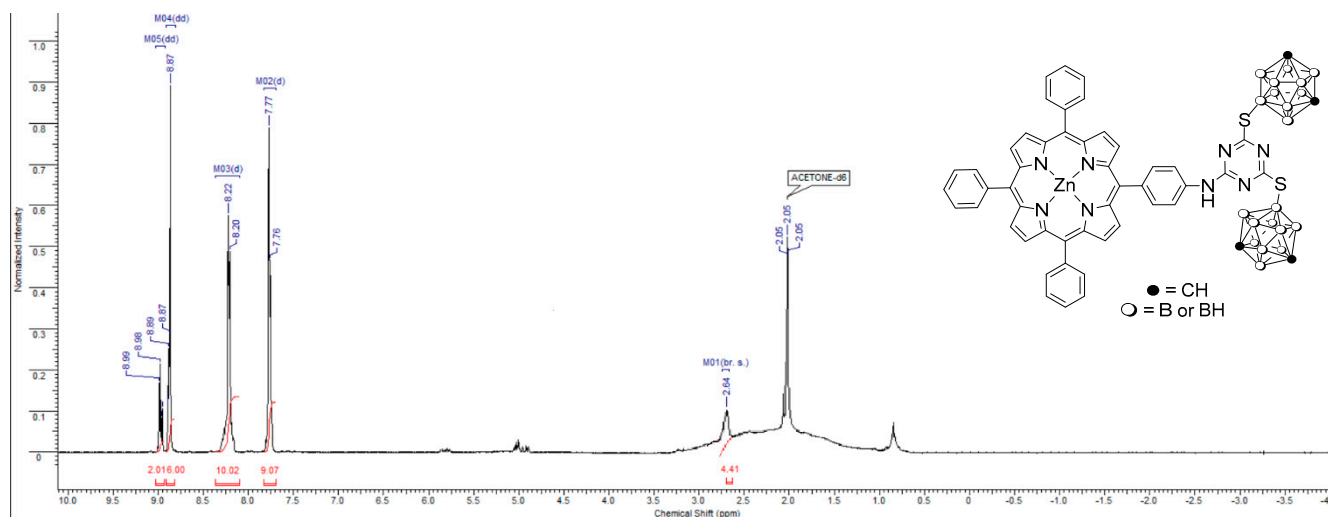
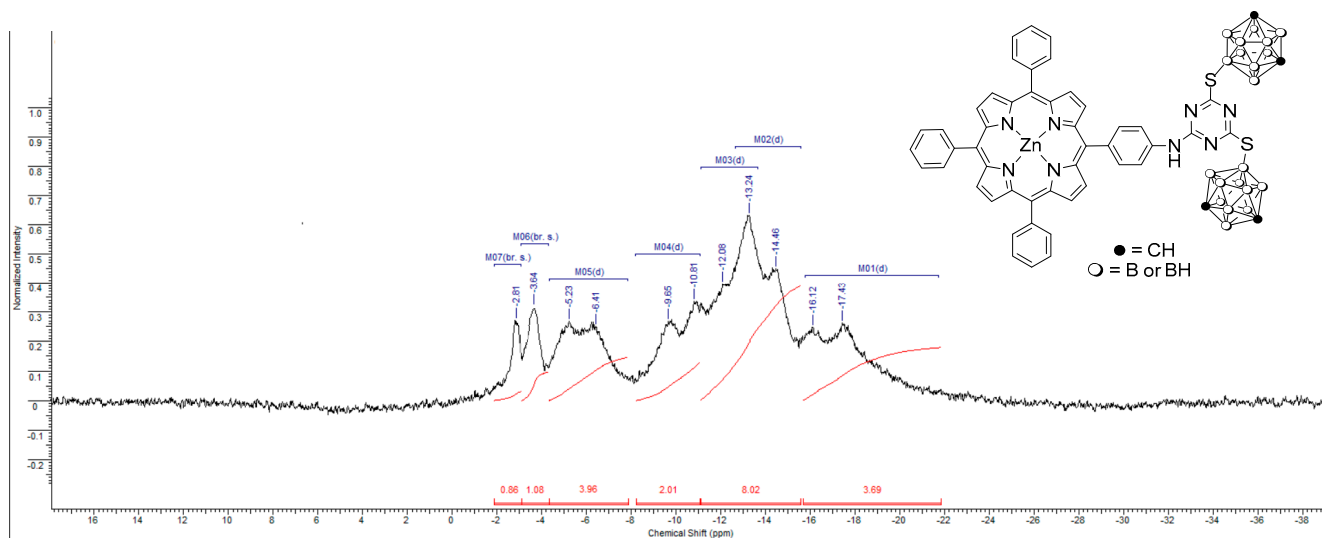


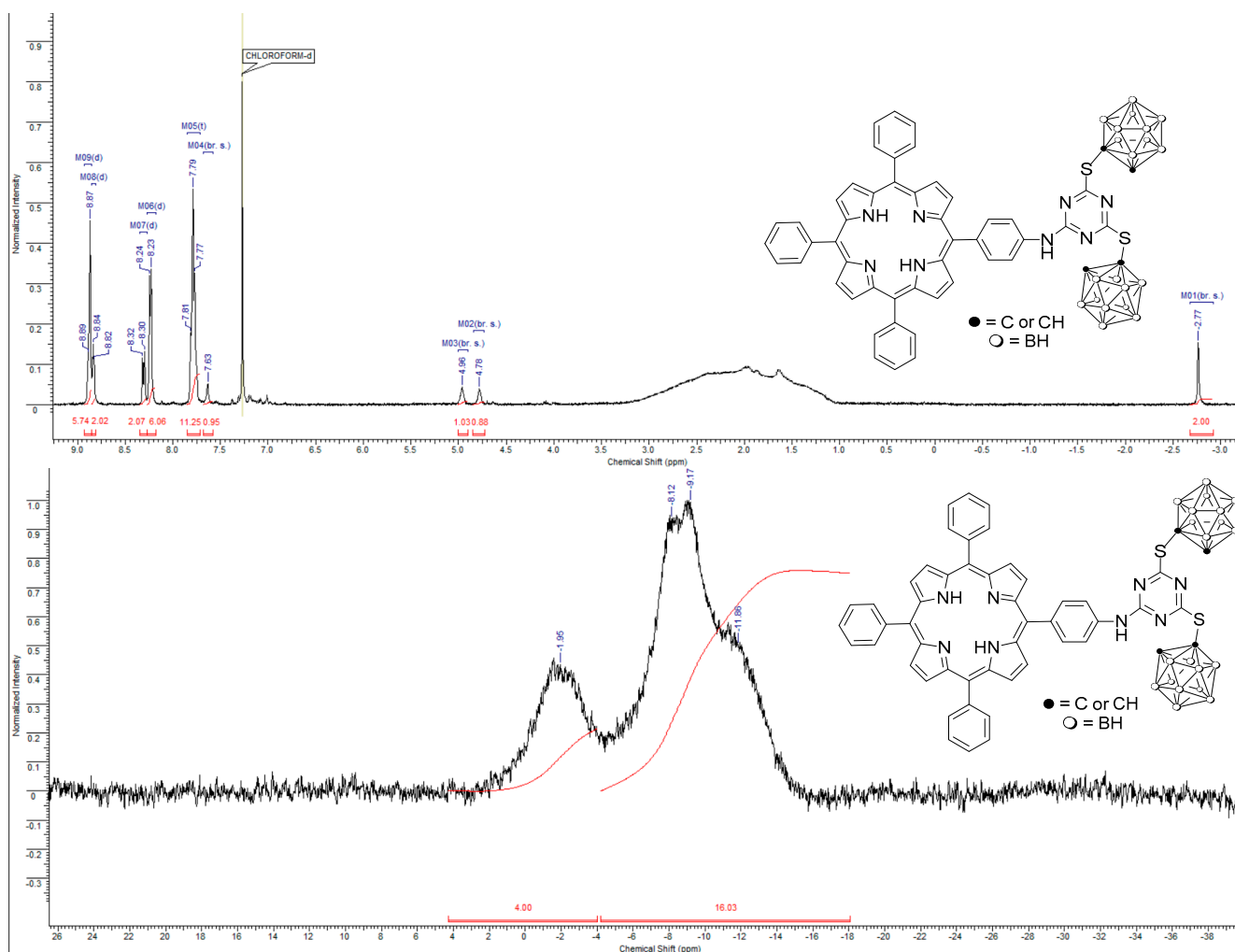
Figure S1. The  $^1\text{H}$ ,  $^{11}\text{B}$  NMR spectra of 5 in  $\text{CDCl}_3$ .

2. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra 5-{4-[[4,6-bis(*m*-carborane-9'-yl)thio]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrinato zinc (II) (6)





### 3. The $^1\text{H}$ and $^{11}\text{B}$ NMR spectra of 5-{4-[[4,6-bis(*o*-carborane-1'-yl)thio]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrin (**8**)



4. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4,6-bis(*o*-carborane-1'-yl)thio]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrinato zinc (II) (**9**)

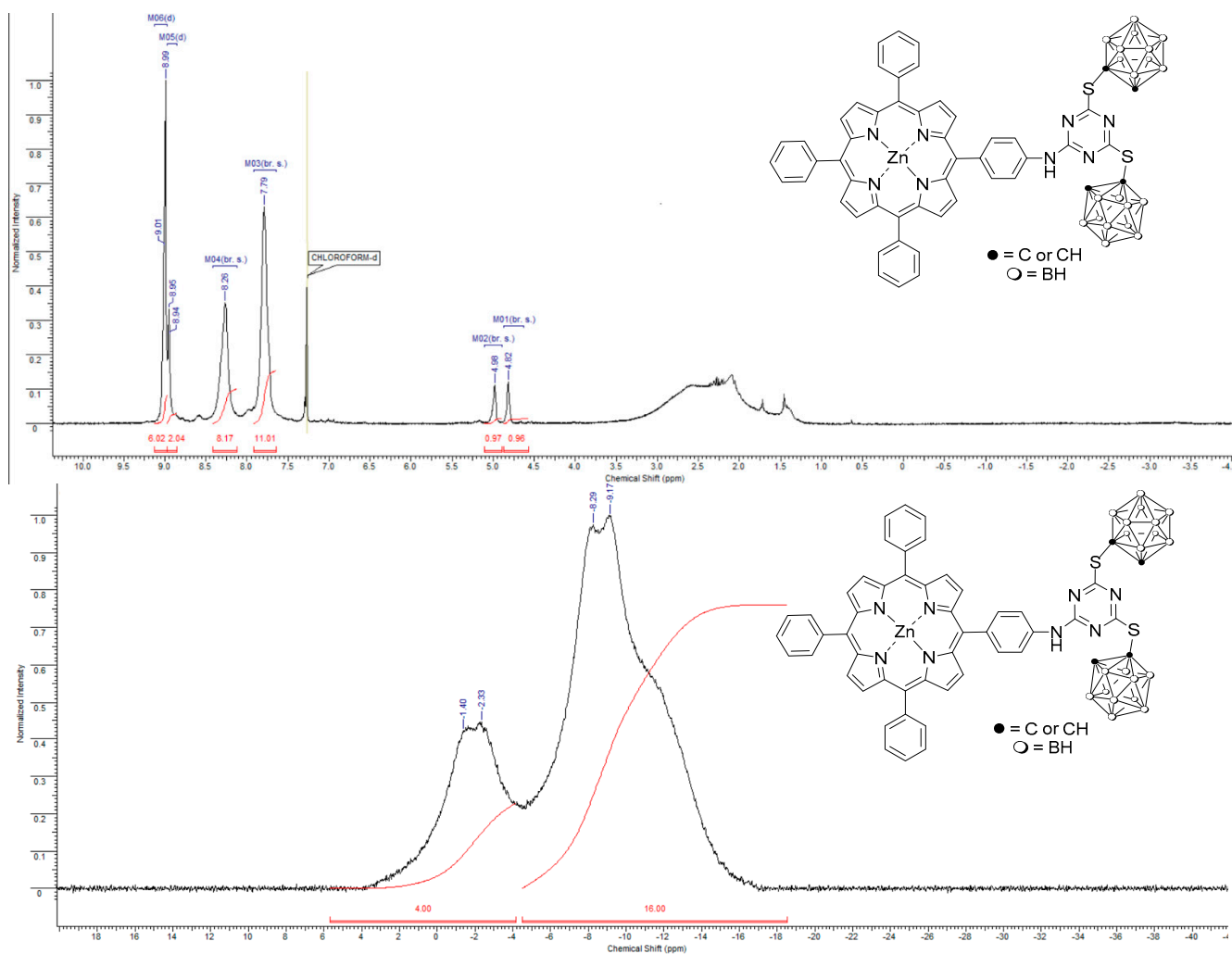
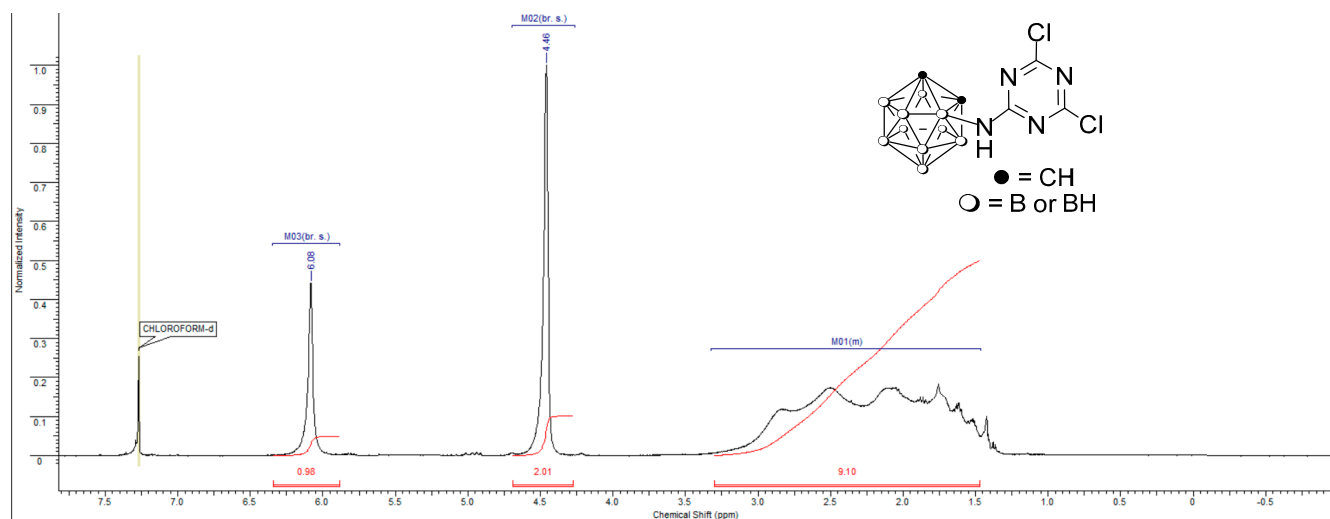


Figure S4. The  $^1\text{H}$ ,  $^{11}\text{B}$  NMR spectra of **9** in  $\text{CDCl}_3$ .

5. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 2-[(*o*-carborane-3'-yl)amino]-4,6-dichloro-(1,3,5)-triazine (**11**)



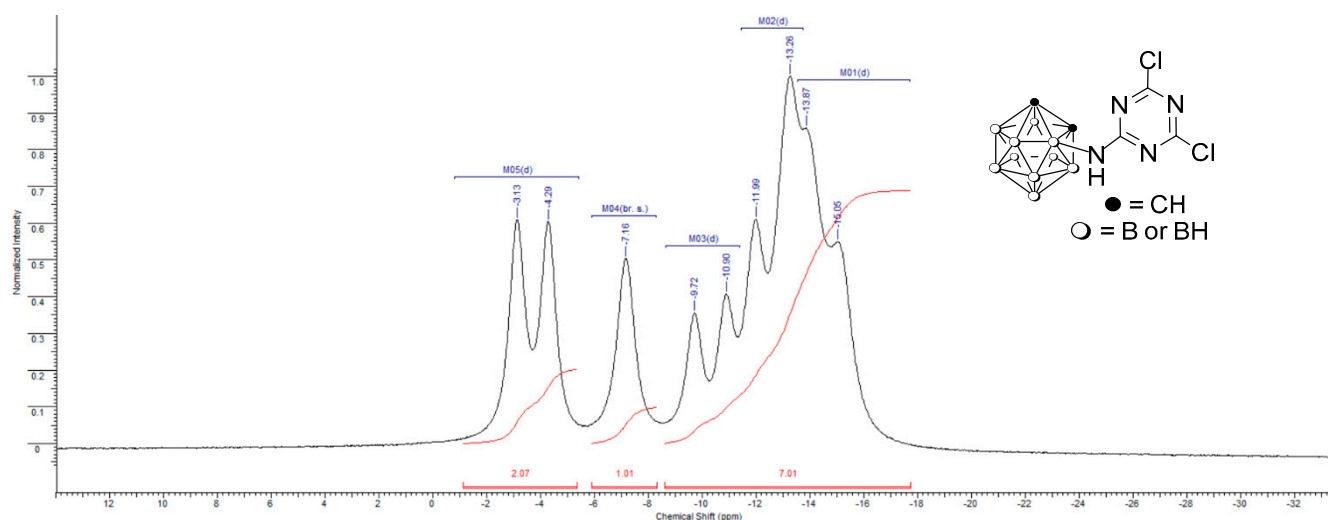


Figure S5. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of **11** in  $\text{CDCl}_3$ .

**6. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-[4-[[4-(*o*-carborane-3'-yl)amino]-6-chloro-(1,3,5)-triazine-2-yl]aminophenyl]-10,15,20-triphenylporphyrin (**12**)**

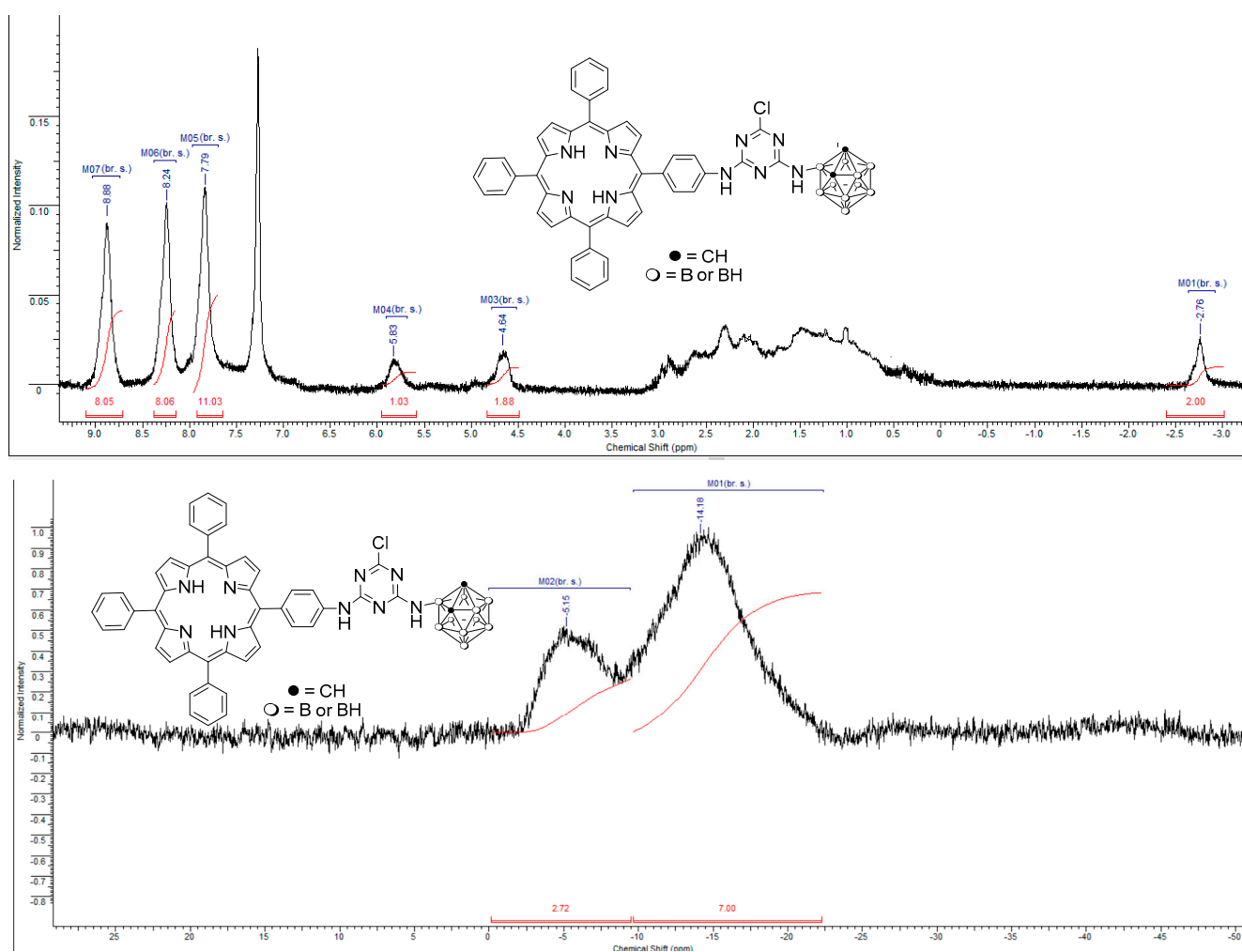


Figure S6. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of **12** in  $\text{CDCl}_3$ .

**7. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4-(*o*-carborane-3'-yl)amino]-(6-carboxymethylthio)-(1,3,5)-triazine-2-yl]-aminophenyl}-10,15,20-triphenylporphyrin (17)**

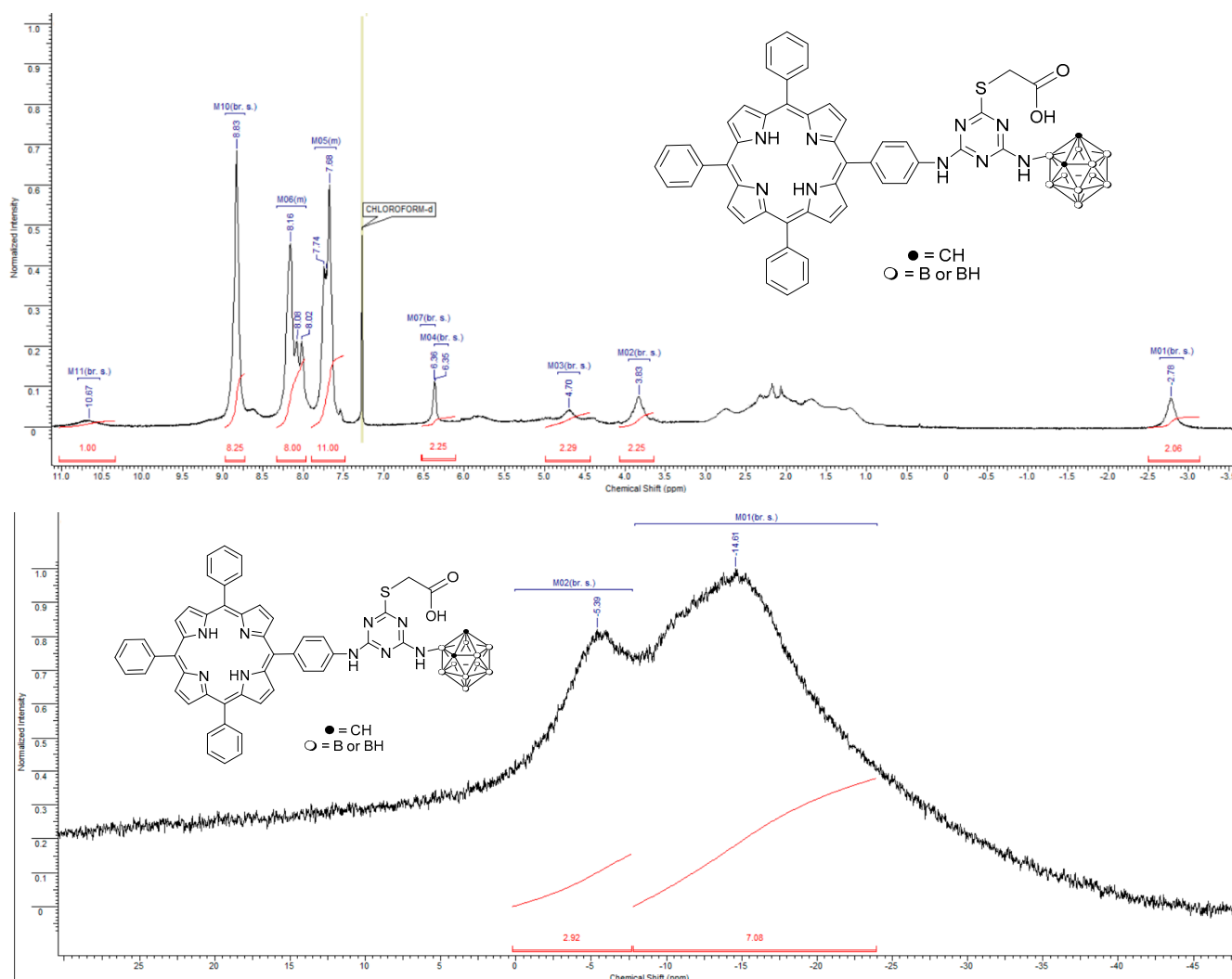
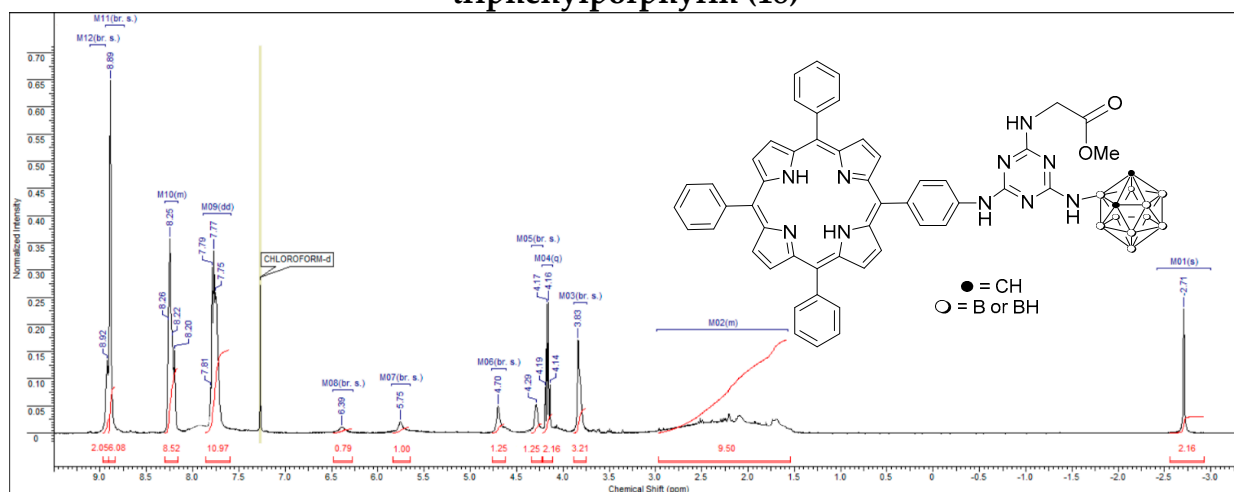


Figure S7. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 17 in  $\text{CDCl}_3$ .

**8. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4-(*o*-carborane-3'-yl)amino]-(6-methoxycarbonylmethylamino)-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrin (18)**



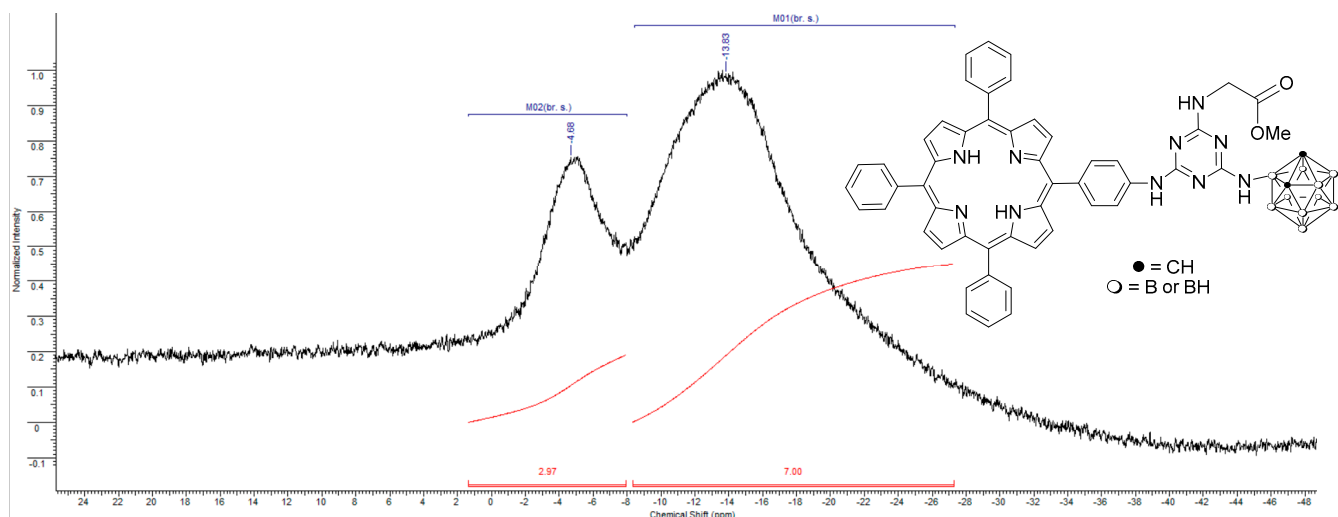


Figure S8. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 18 in  $\text{CDCl}_3$ .

9. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4-(*o*-carborane-3'-yl)amino]-[6-((2-hydroxyethyl)thio)]-(1,3,5)-triazine-2-yl]-aminophenyl]-10,15,20-triphenylporphyrin (19)

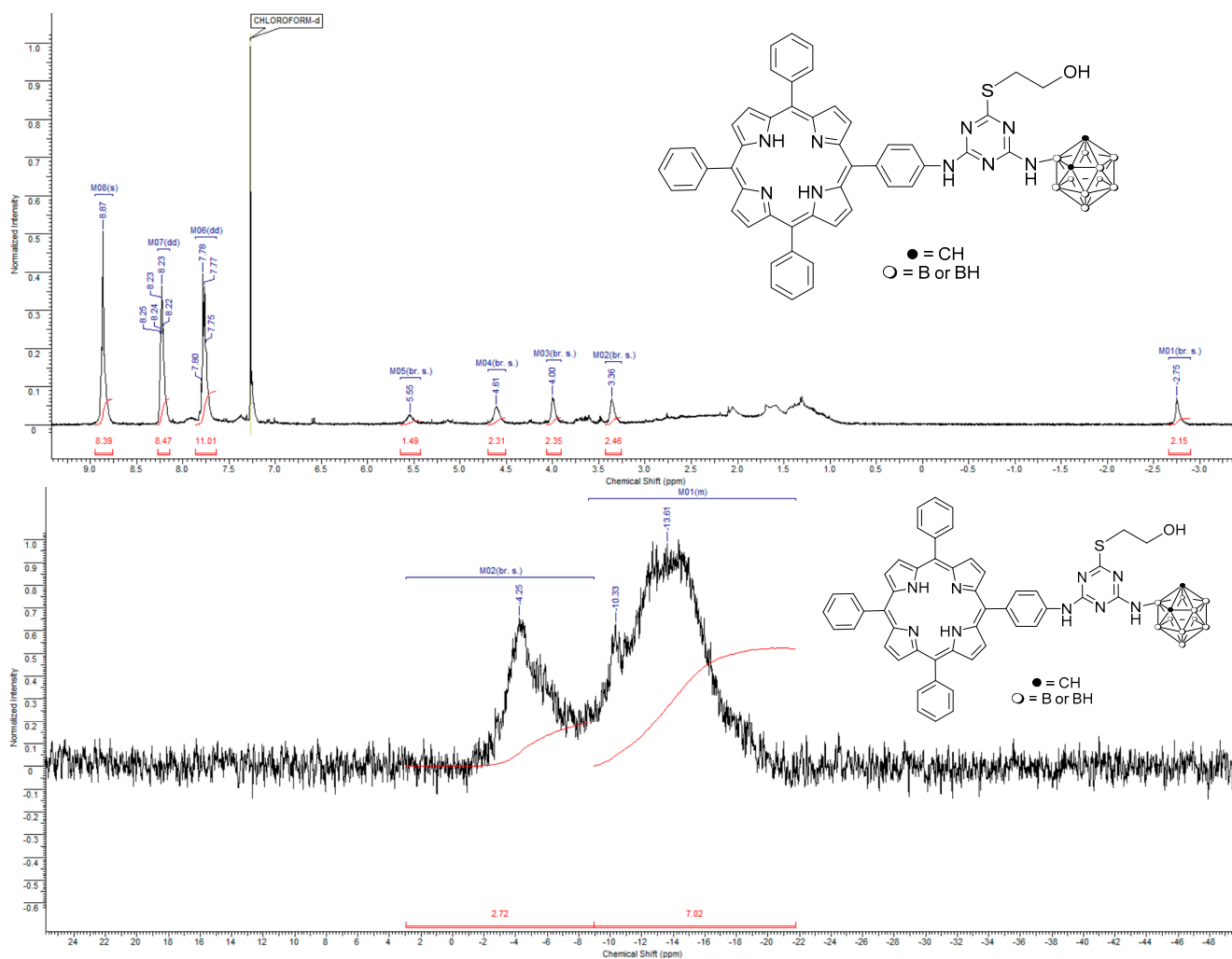
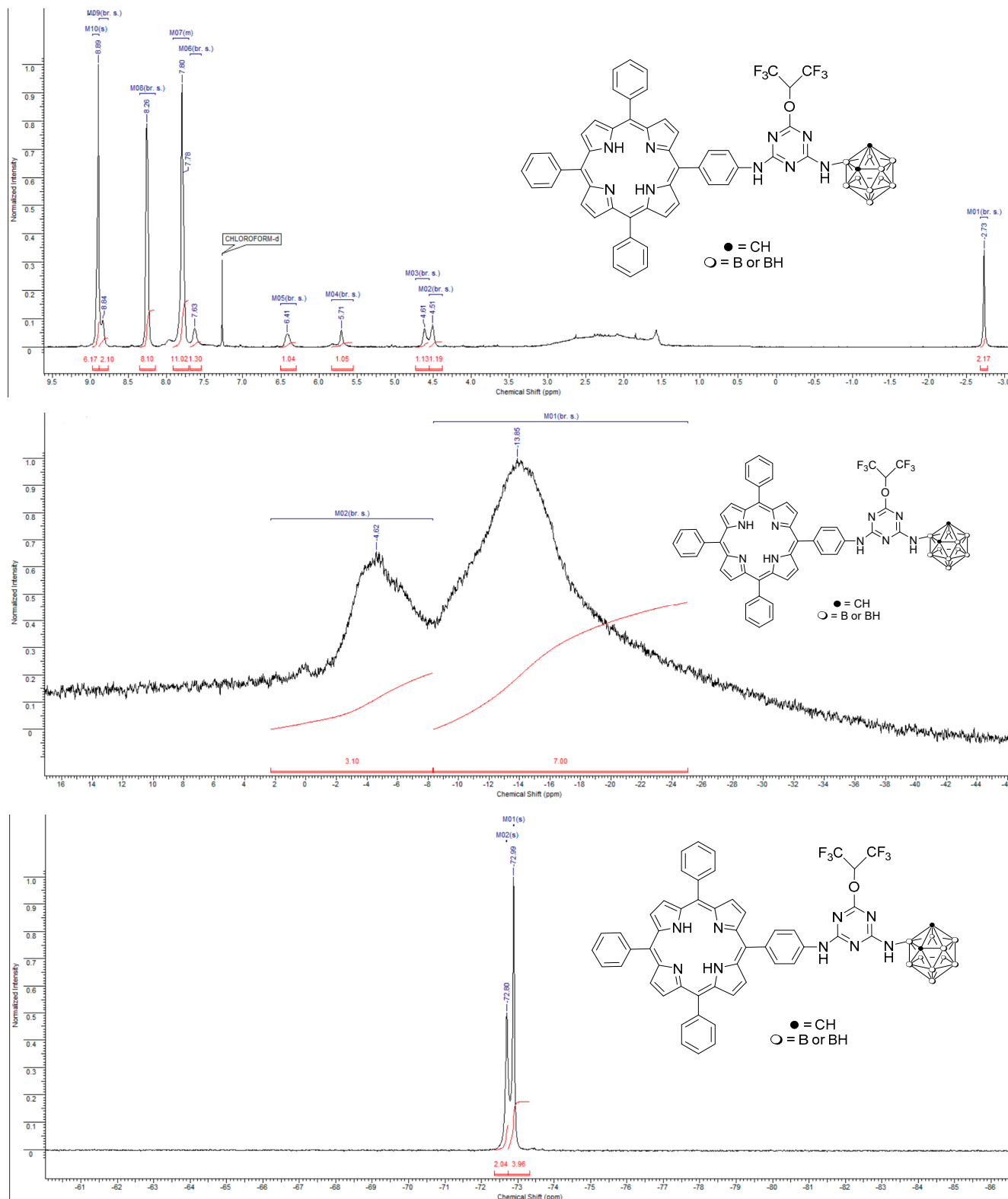


Figure S9. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 19 in  $\text{CDCl}_3$ .



**10. The  $^1\text{H}$ ,  $^{11}\text{B}$  and  $^{19}\text{F}$  NMR spectra of 5-{4-[[4-(*o*-carborane-3'-yl)amino]-[6-(1,1,1,3,3,3-hexafluoro-propan-2-yl)oxy]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrin (**20**)**



**Figure S10.** The  $^1\text{H}$ ,  $^{11}\text{B}$  and  $^{19}\text{F}$  spectra of **20** in  $\text{CDCl}_3$ .

**11. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4-(*m*-carborane-9'-yl)thio]-[6-(aminoethylthio)]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrin (**21**)**

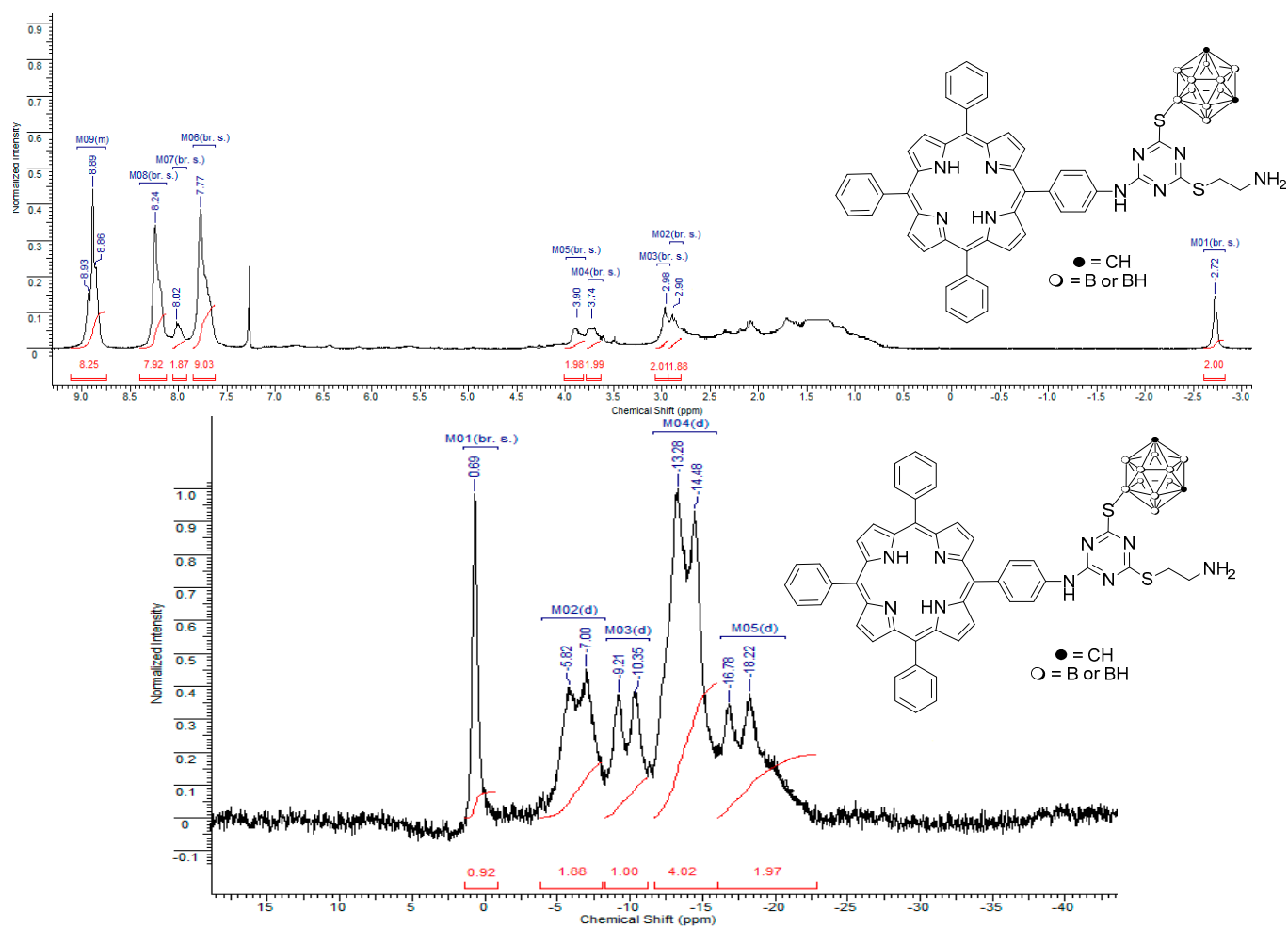
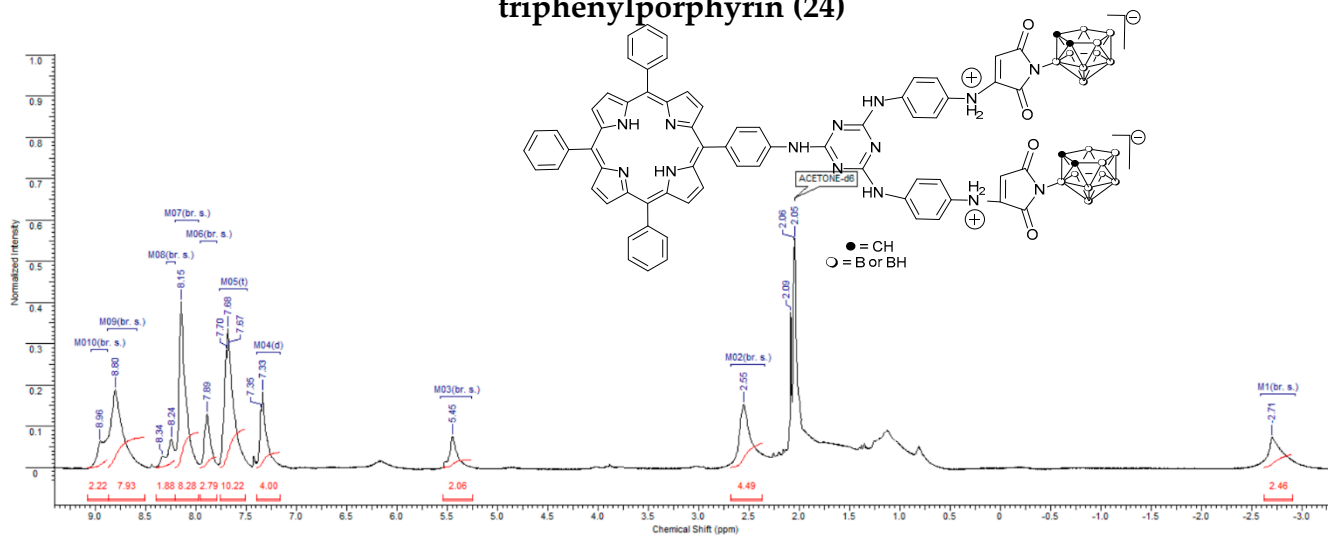


Figure S11. The  $^1\text{H}$ ,  $^{11}\text{B}$  NMR spectra of **21** in  $\text{CDCl}_3$ .

**12. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4,6-bis((4-(1-(*N*-(7,8-dicarbaundecaborate-3'-yl))maleimido)aminophenyl)-amino]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrin (**24**)**



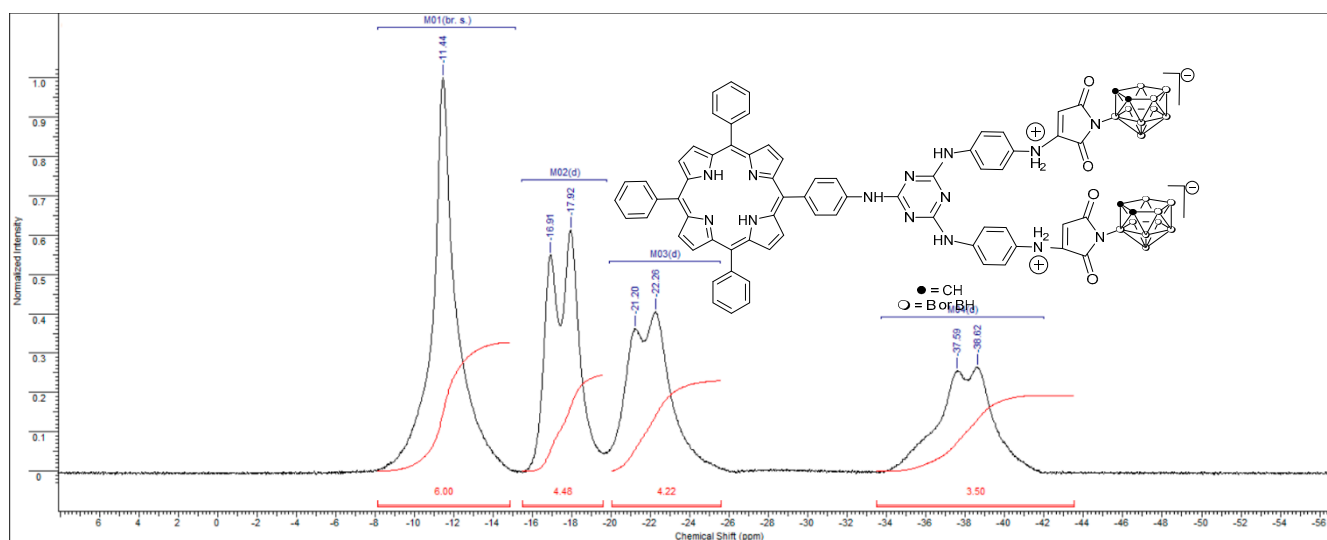


Figure S12. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of **24** in  $(\text{CD}_3)_2\text{CO}$ .

**13. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of 5-{4-[[4,6-bis((4-(1-(*o*-carborane-3'-yl))maleimido)aminophenyl)amino]-(1,3,5)-triazine-2-yl]aminophenyl}-10,15,20-triphenylporphyrin (**25**)**

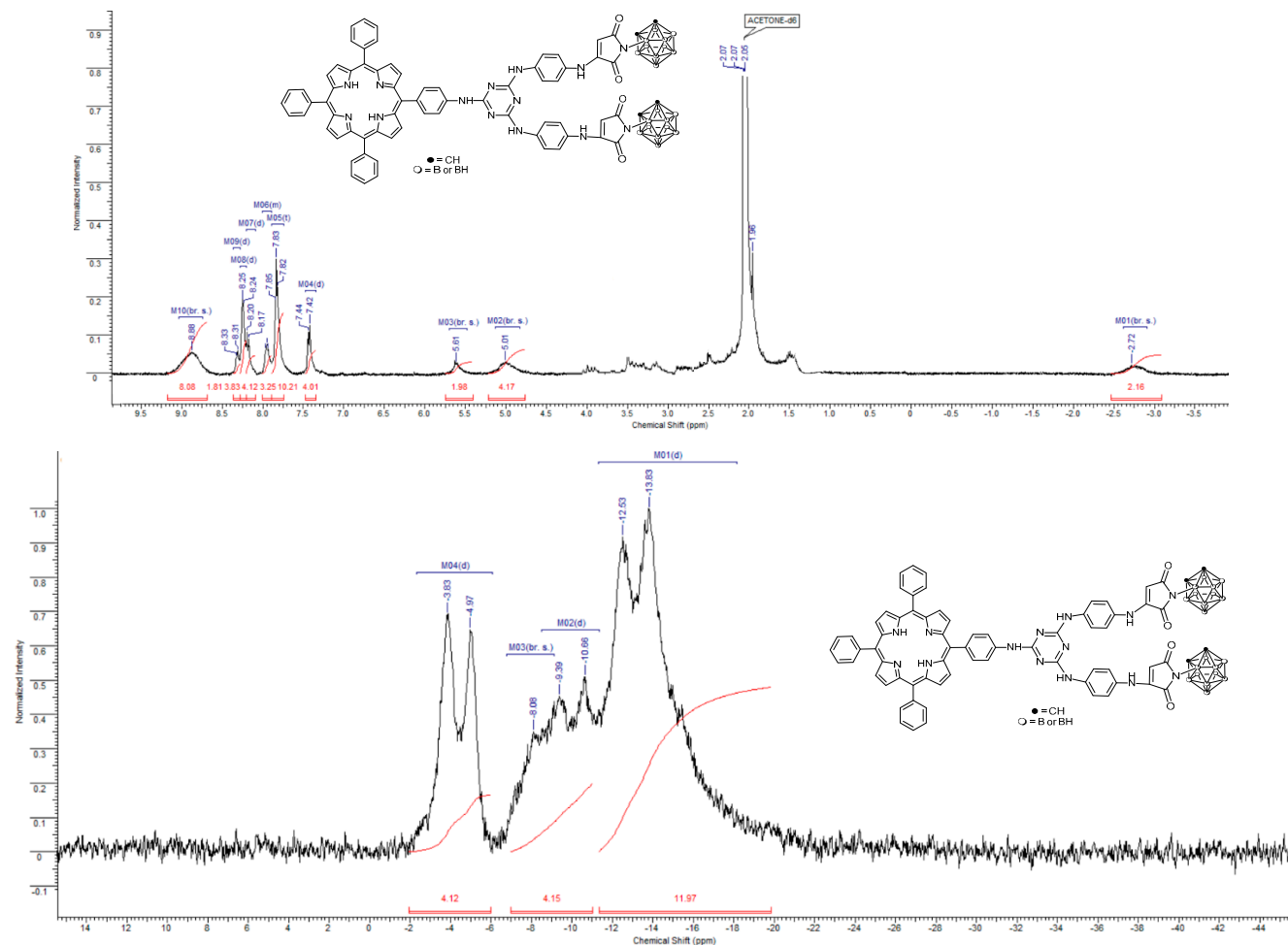


Figure S13. The  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra of **25** in  $(\text{CD}_3)_2\text{CO}$ .

#### 14. The dark cytotoxicity of carboranylporphyrins 8, 9, 17, 18 and 24

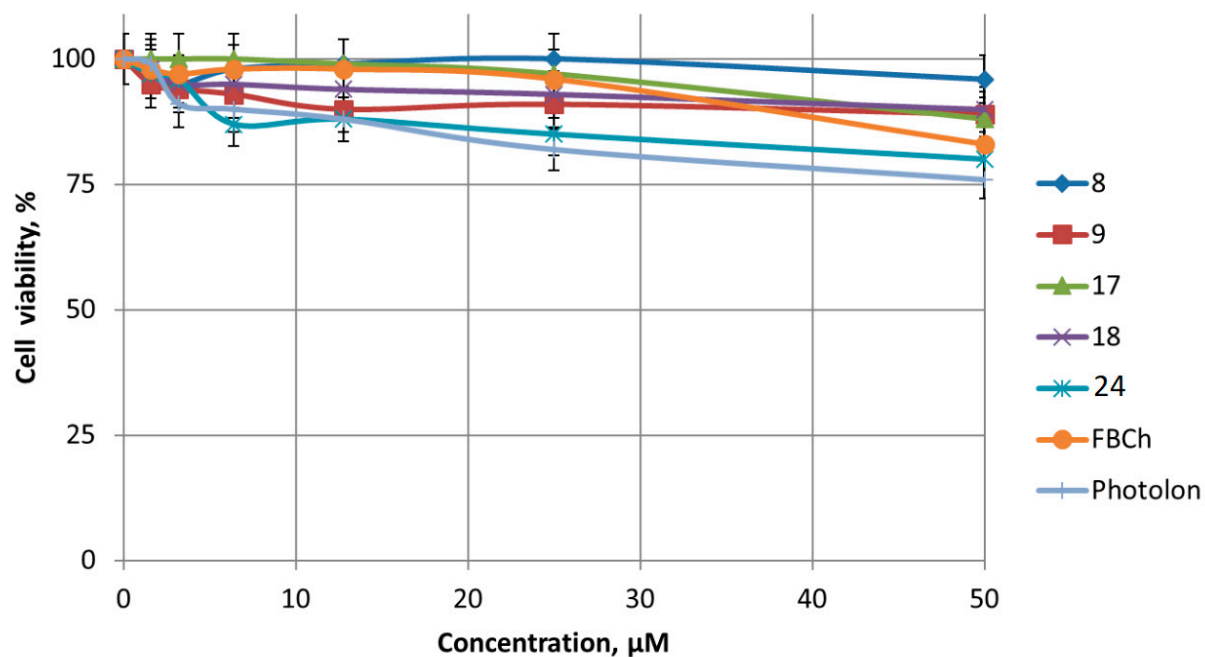


Figure S14. Dark cytotoxicity of compounds 8, 9, 17, 18 and 24.

#### 15. The photoinduced cytotoxicity of carboranylporphyrins 8, 9, 17, 18 and 24

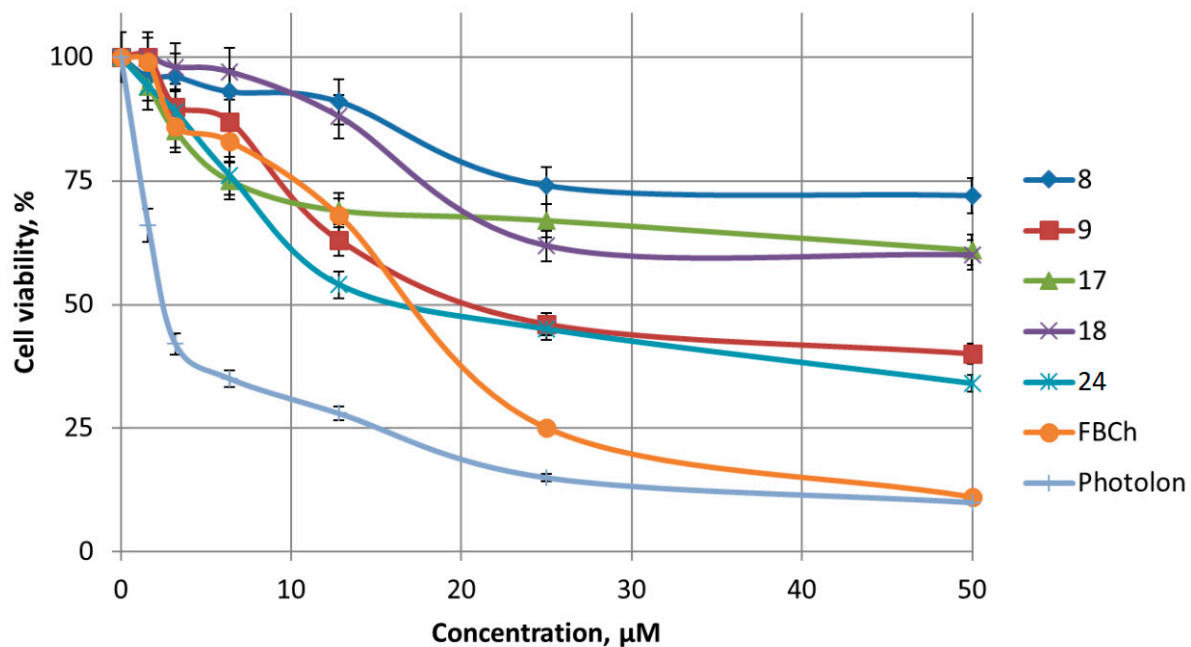


Figure S15. Photoinduced cytotoxicity of compounds 8, 9, 17, 18 and 24.