**Supporting Information**

# Epidermal Growth Factor Receptor Targeted Multifunctional Photosensitizers for Bladder Cancer Imaging and Photodynamic Therapy

Ravindra R. Cheruku, Joseph Cacaccio, Farukh A. Durrani, Walter A. Tabaczynski, Ramona Watson, Aimee Marko, Rahul Kumar, Mohamed E. El-Khouly, Shunichi Fukuzumi, , Joseph R. Missert, Rutao Yao, Munawwar Sajjad, Dhyan Chandra, Khurshid Guru and Ravindra K Pandey*

**Contents:**

**Figure S1**: $^{1}$H-NMR (400 MHz, $CDCl_3$)



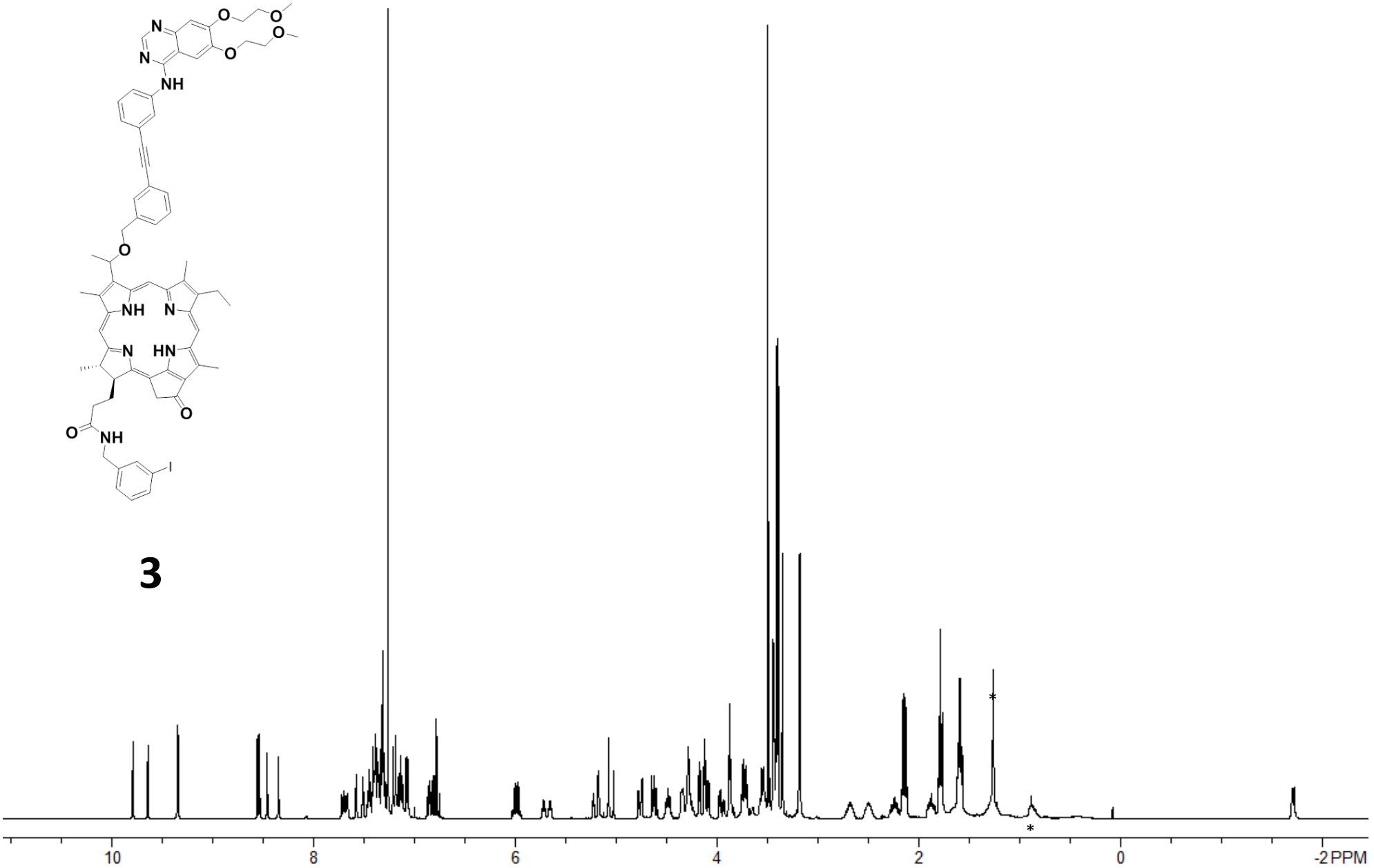
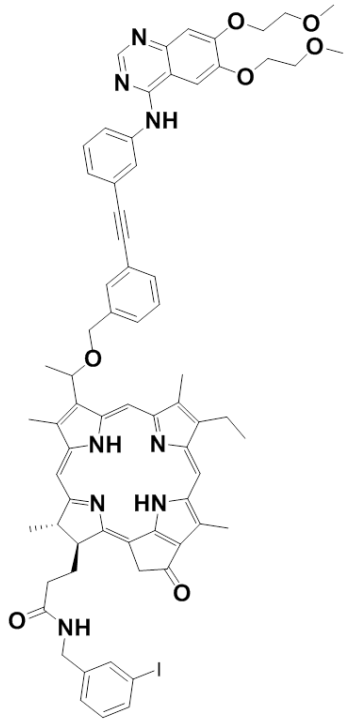


**Figure S2:** $^{13}$C-NMR (100 MHz, $CDCl_3$)





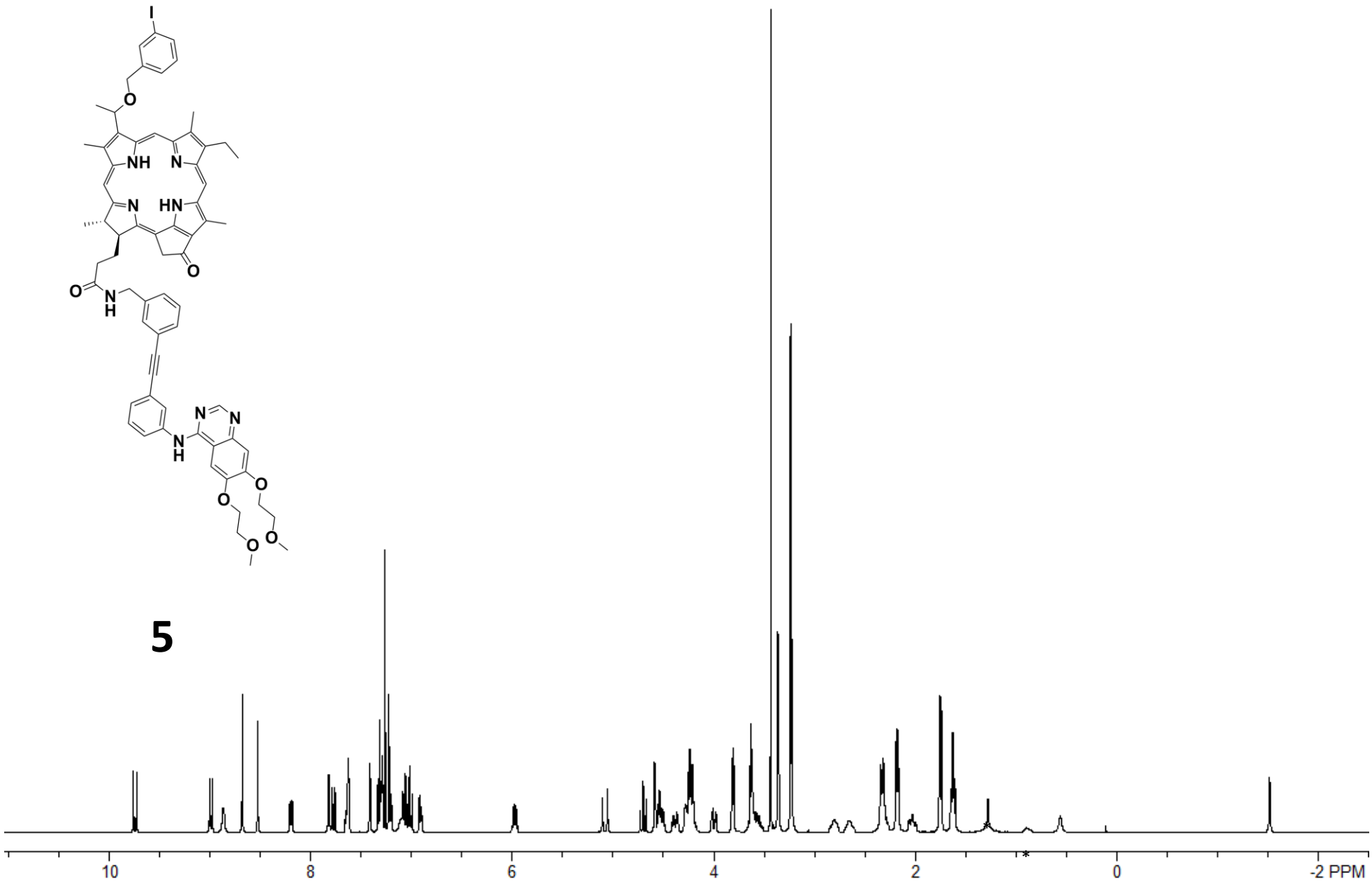
**3**




* Grease impurity

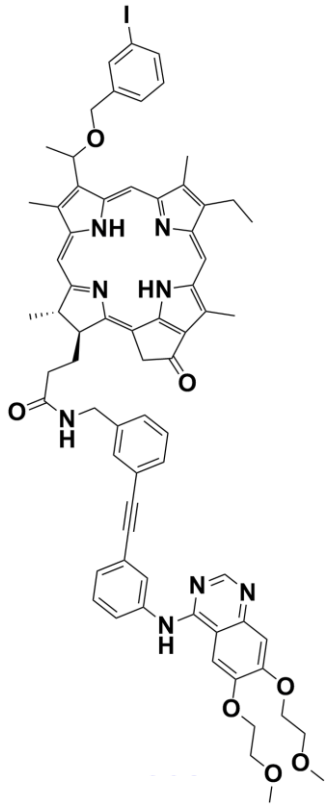
**Figure S3**: $^{1}$H-NMR (400 MHz, $CDCl_3$)






* Grease impurity

**Figure S4**: $^{13}$C-NMR (100 MHz, $CDCl_3$)



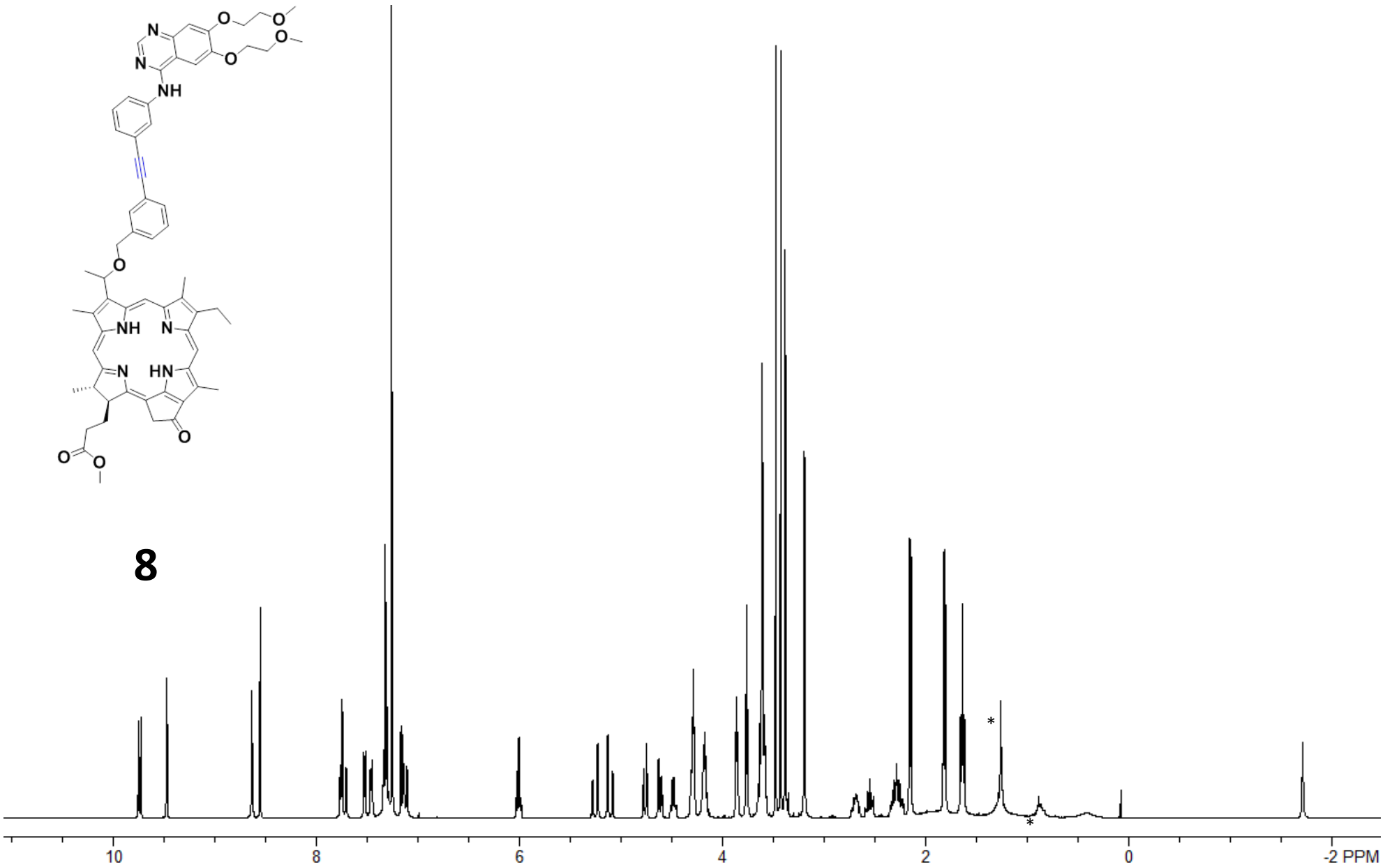
**5**




* Grease impurity

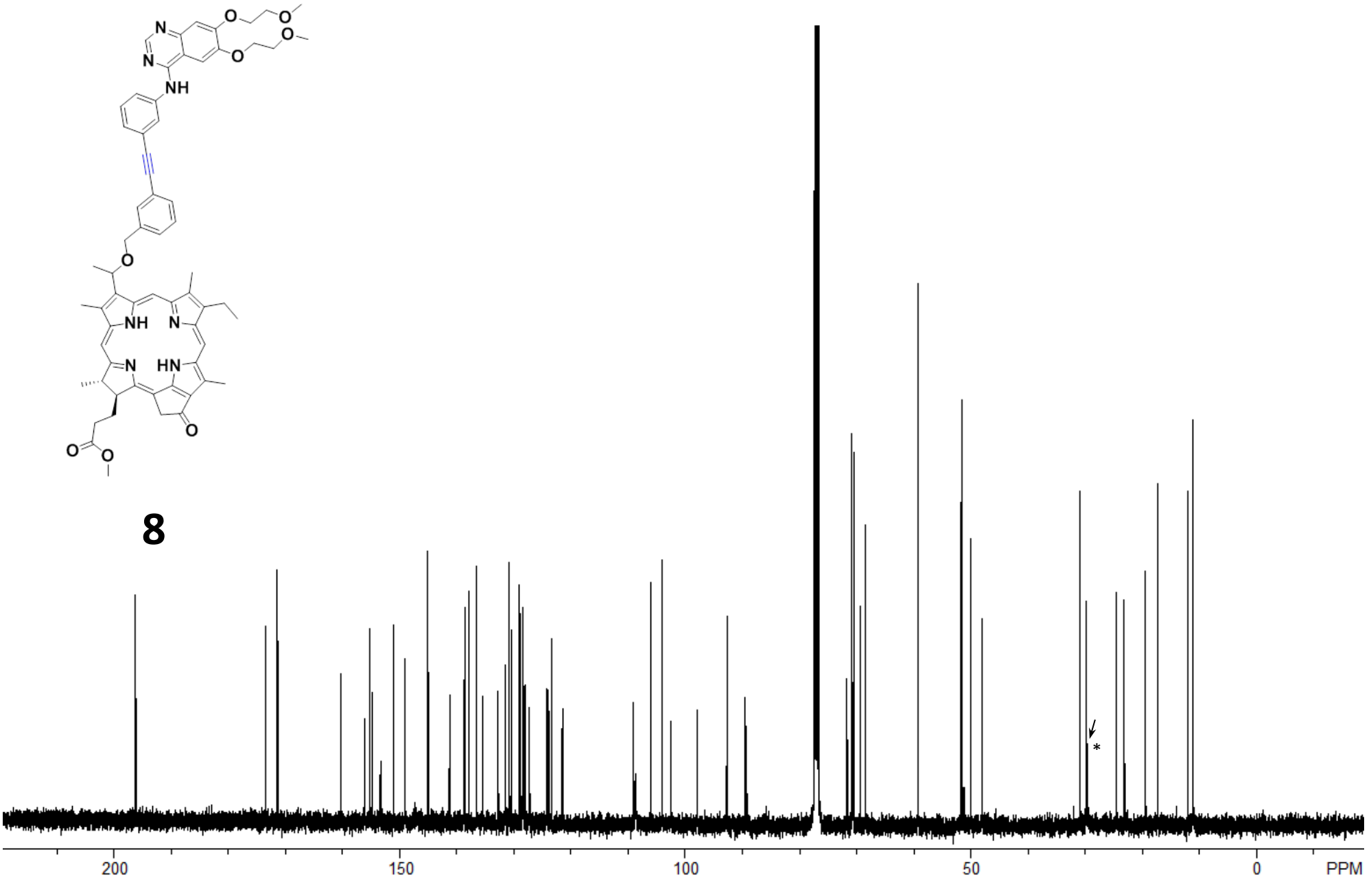
**Figure S5**: $^{1}$H-NMR (400 MHz, $CDCl_3$)






* Grease impurity

**Figure S6:** $^{13}$C-NMR (100 MHz, $CDCl_3$)




* Grease impurity

**Figure S7:** $^{1}$H-NMR (400 MHz, 90:10 $CDCl_3/CD_3OD$)



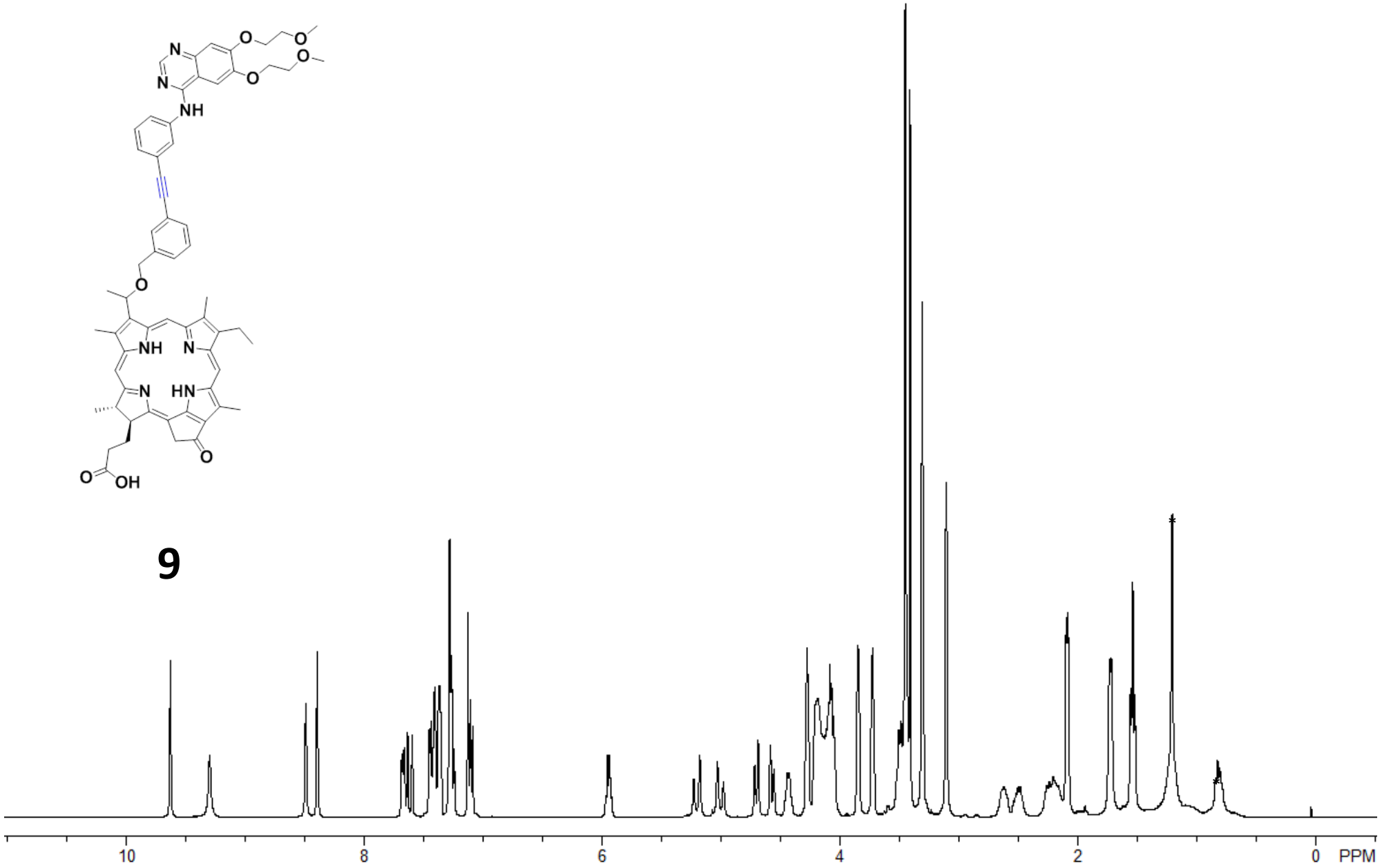
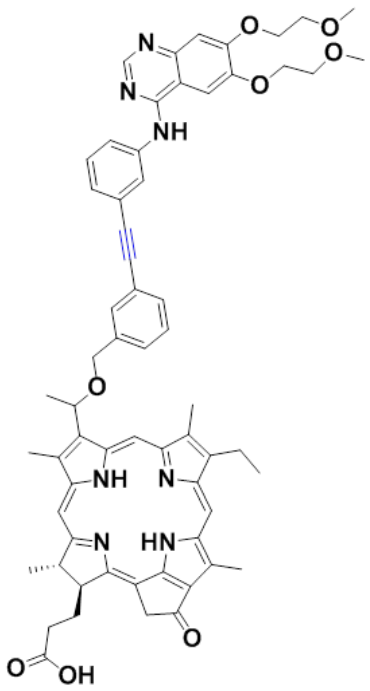


**Figure S8:** $^{13}$C-NMR (100 MHz, 90:10 $CDCl_3$/$CD_3OD$)





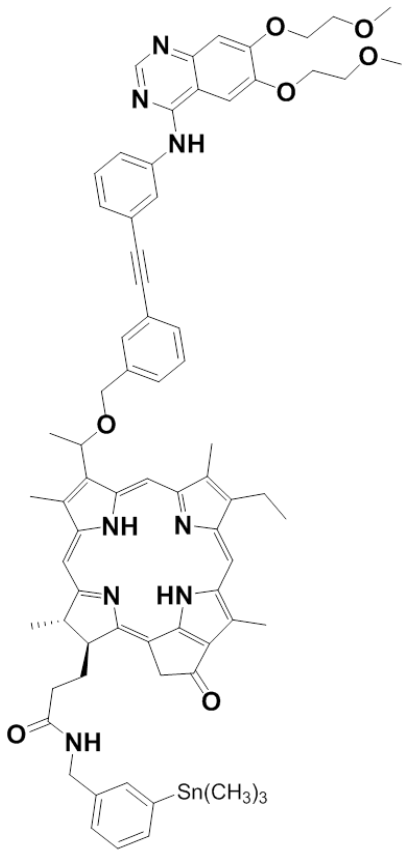
**9**




* Grease impurity

**Figure S9:** $^{1}$H-NMR (400 MHz, $CDCl_3$)





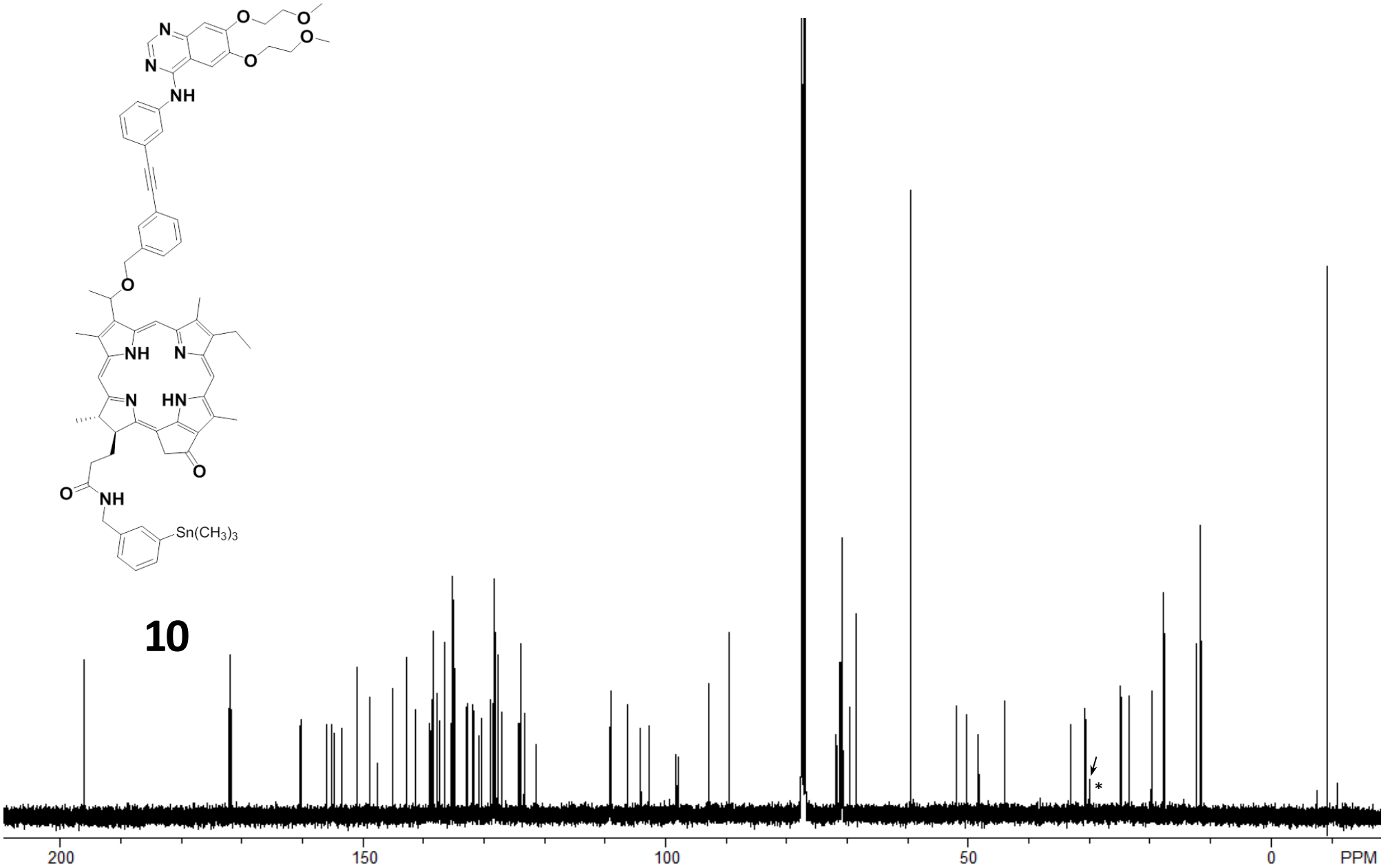

**10**




* Grease impurity

**Figure S10:** $^{13}$C-NMR (100 MHz, $CDCl_3$)

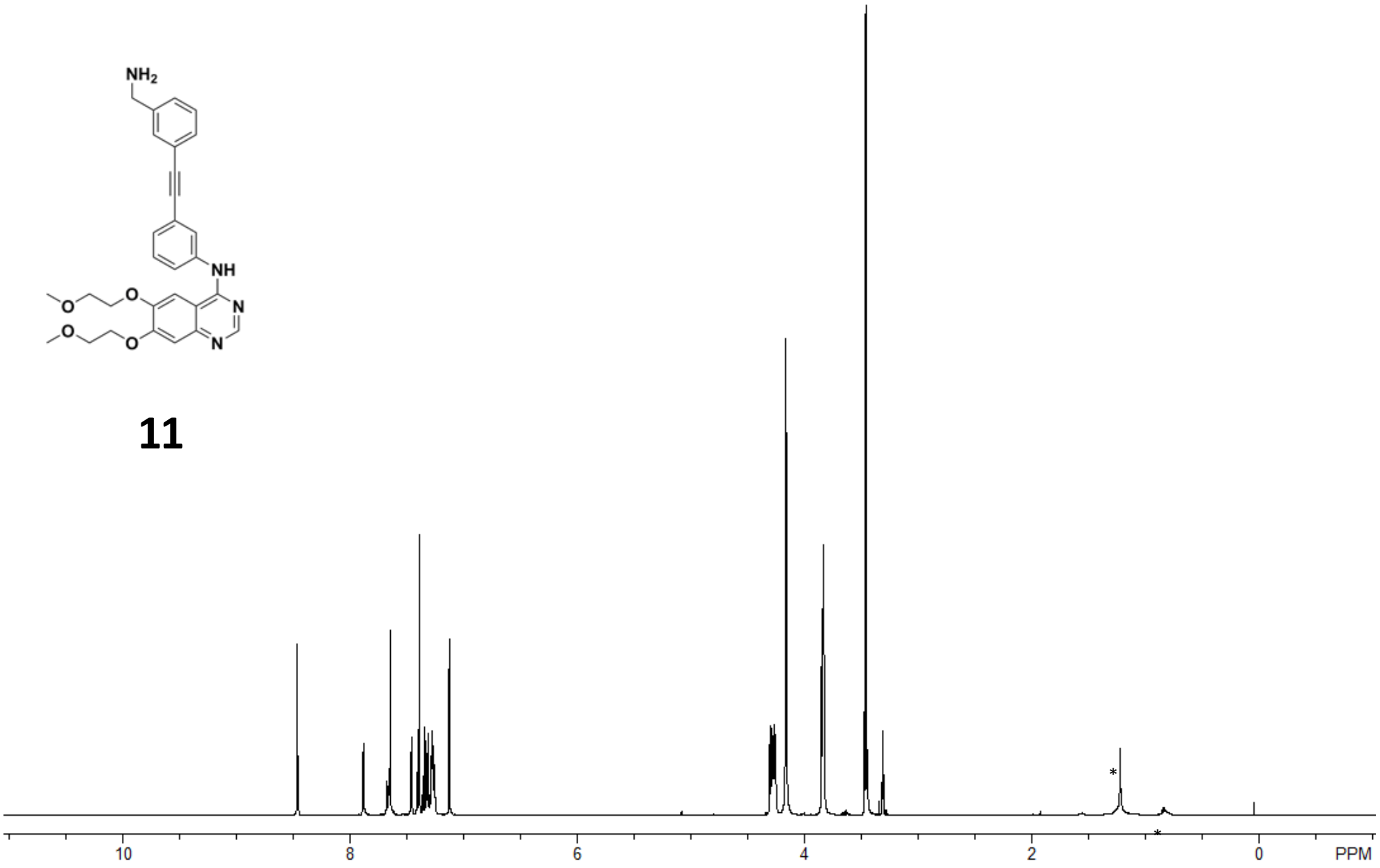





* Grease impurity

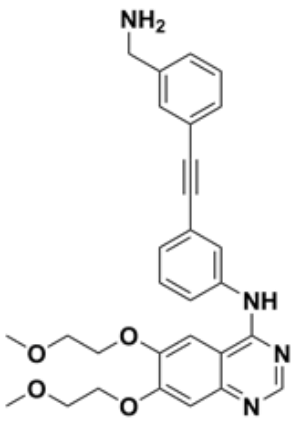
**Figure S11**: $^1$H-NMR (400 MHz, 80:20 $CDCl_3/CD_3OD$)






* Grease impurity

**Figure S12**: $^{13}$C-NMR (100 MHz, 80:20 $CDCl_3$/$CD_3OD$)



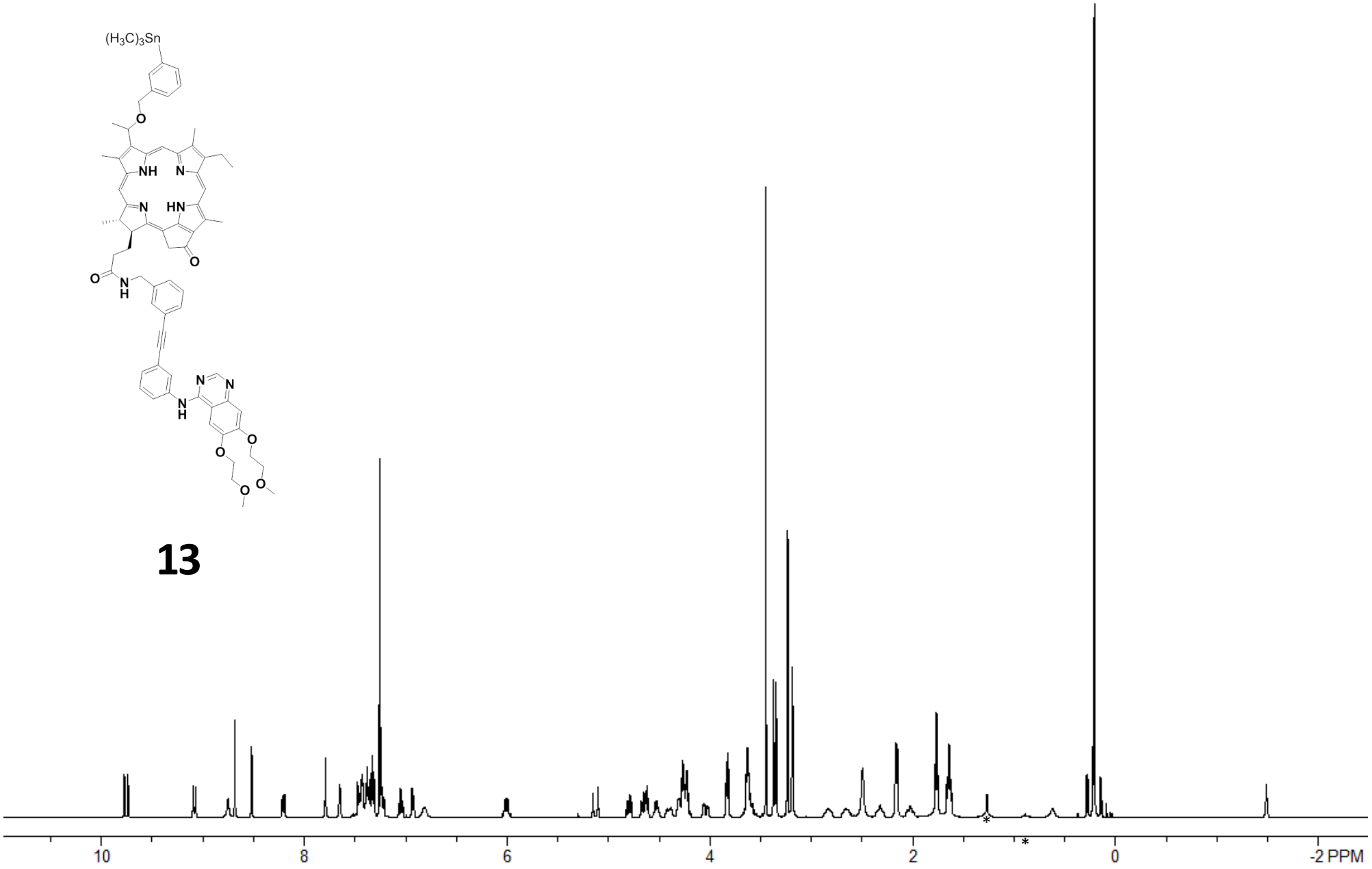

**11**




* Grease impurity

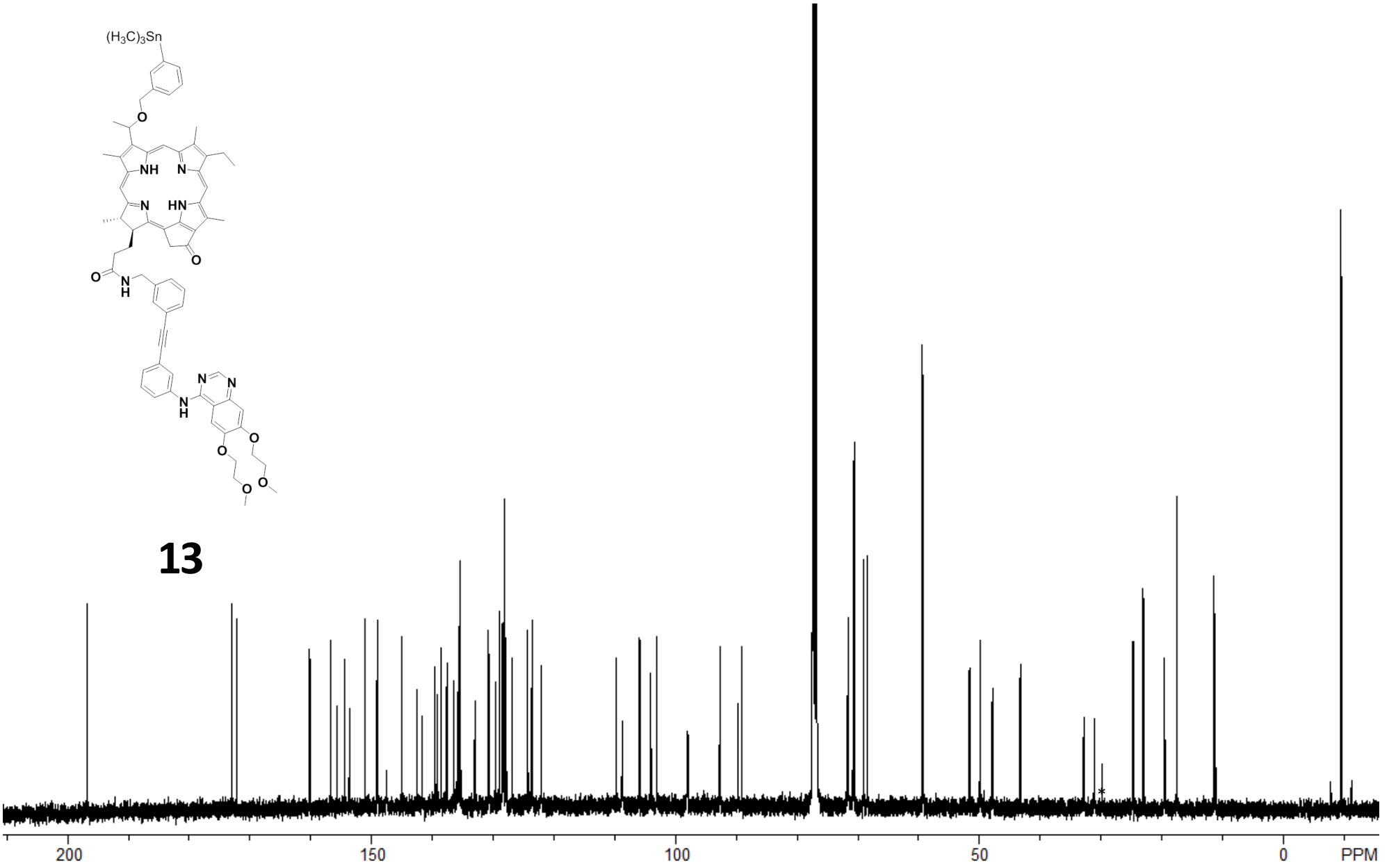
**Figure S13:** $^{1}$H-NMR (400 MHz, $CDCl_3$)






* Grease impurity

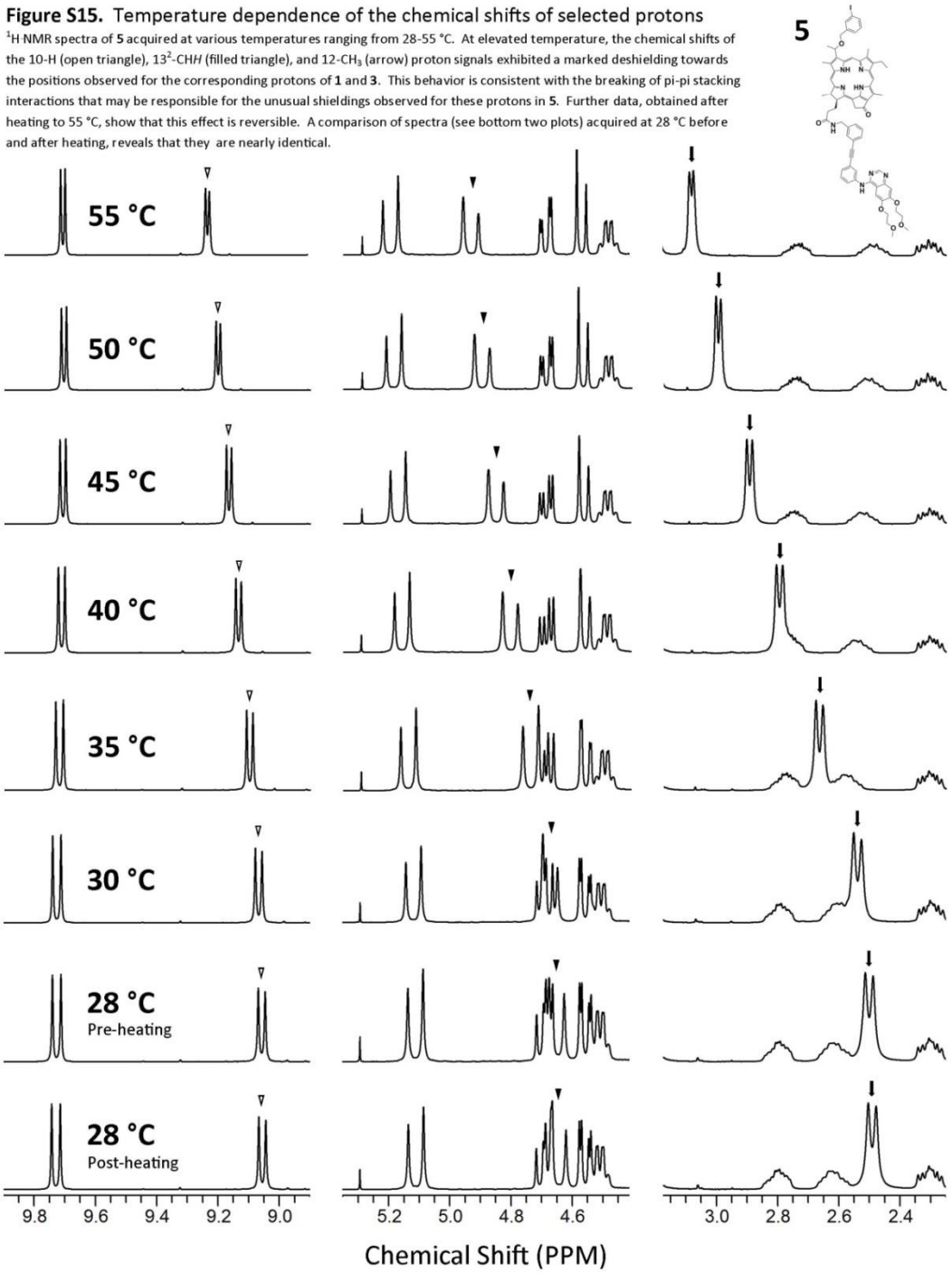
**Figure S14**: $^{13}$C-NMR (100 MHz, $CDCl_3$)




* Grease impurity

**Figure S15.** Temperature dependence of the chemical shifts of selected protons

$^1$H NMR spectra of **5** acquired at various temperatures ranging from 28-55 °C. At elevated temperature, the chemical shifts of the 10-H (open triangle), 13$^2$-CH*H* (filled triangle), and 12-$CH_3$ (arrow) proton signals exhibited a marked deshielding towards the positions observed for the corresponding protons of **1** and **3**. This behavior is consistent with the breaking of pi-pi stacking interactions that may be responsible for the unusual shieldings observed for these protons in **5**. Further data, obtained after heating to 55 °C, show that this effect is reversible. A comparison of spectra (see bottom two plots) acquired at 28 °C before and after heating, reveals that they are nearly identical.



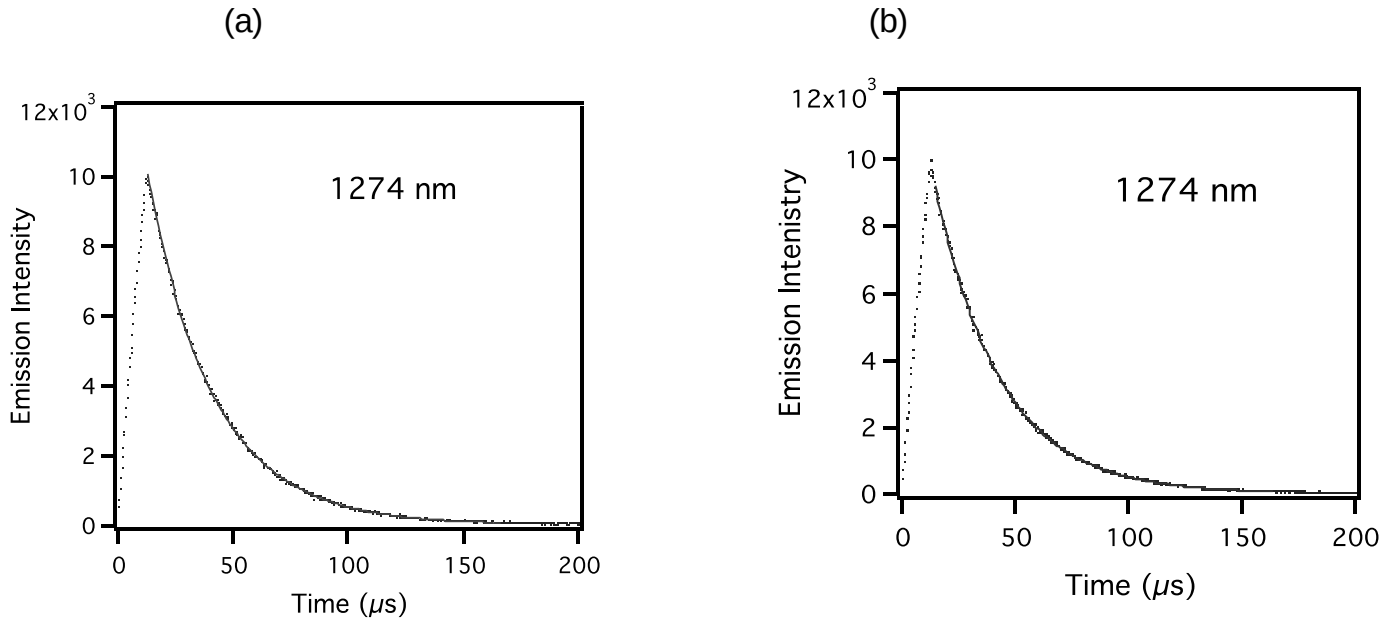



**Figure S16.** Lifetimes of the singlet oxygen in toluene for **3** (a), and **5** (b); $\lambda_{ex}$ = 470 nm.

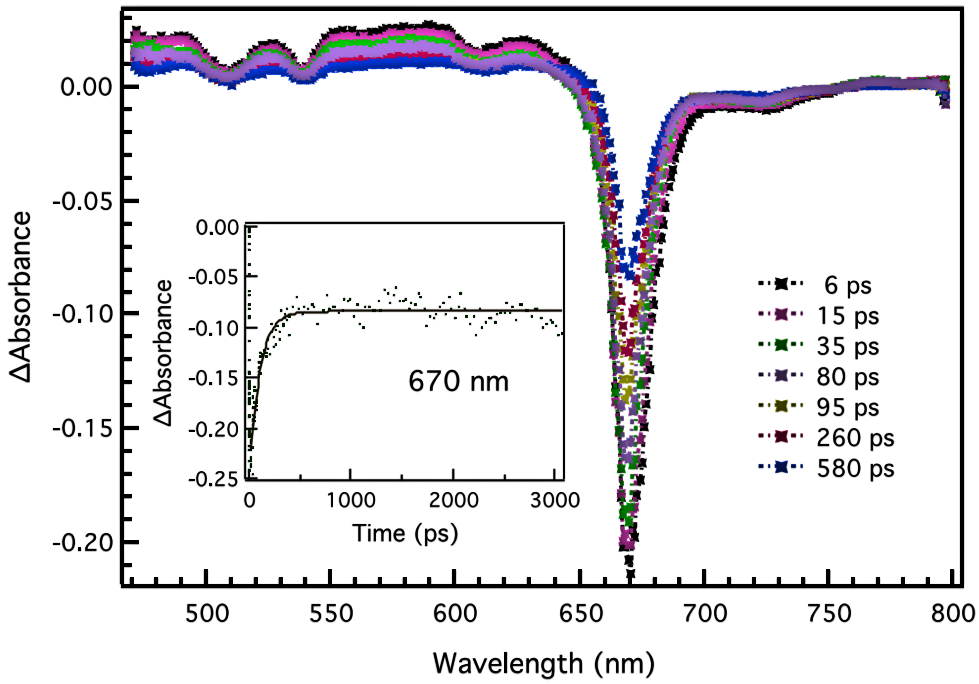



**Figure S17.** Differential absorption spectra obtained upon femtosecond flash photolysis ($\lambda_{ex}$ = 390 nm) of **3** in deaerated touene at the indicated time intervals. The inset shows the time profile of the singlet-excited state at 670 nm.

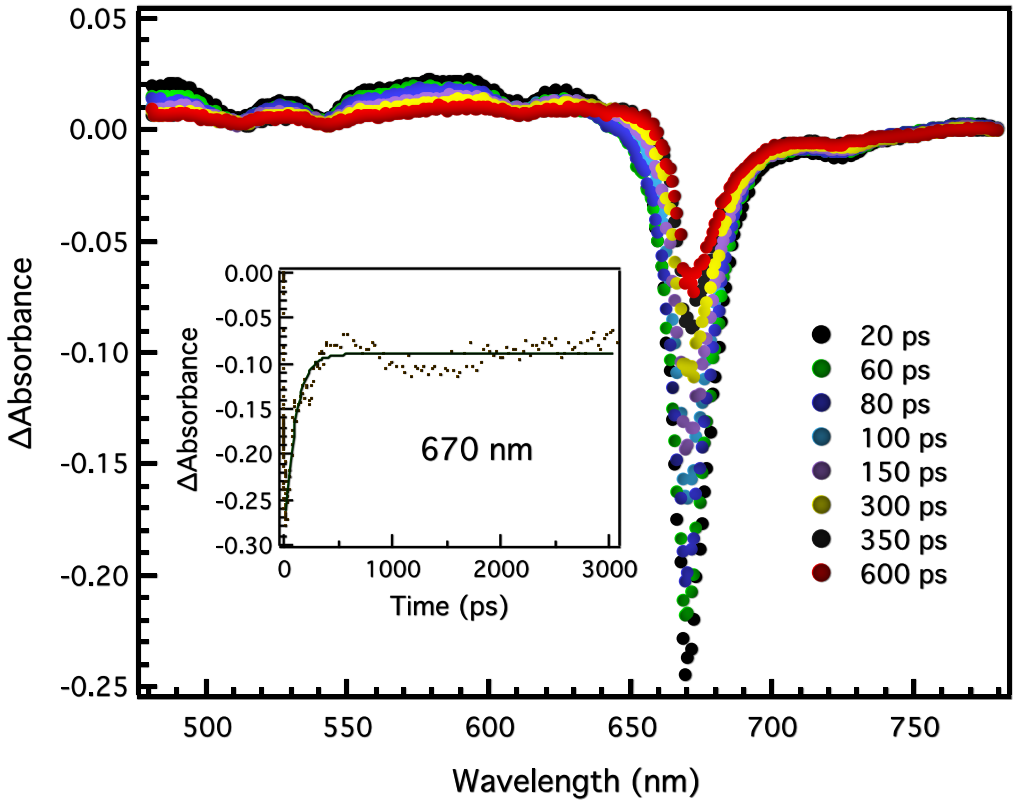



**Figure S18.** Differential absorption spectra obtained upon femtosecond flash photolysis ($\lambda_{ex}$ = 390 nm) of **5** in deaerated touene at the indicated time intervals. The inset shows the time profiles of the singlet-excited state at 670 nm.

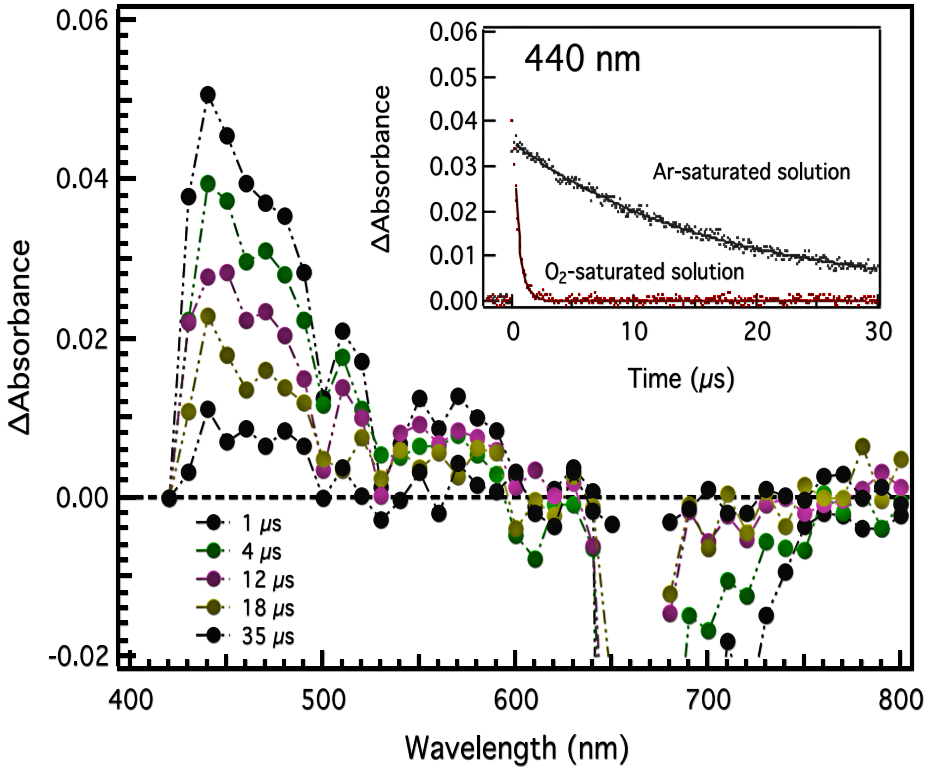



**Figure S19.** Nanosecond transient absorption spectra at the indicated time intervals of PS **1** in Ar-saturated toluene solution. Inset shows the decay profile of the triplet **1** in Ar-saturated and oxygen-saturated solutions.

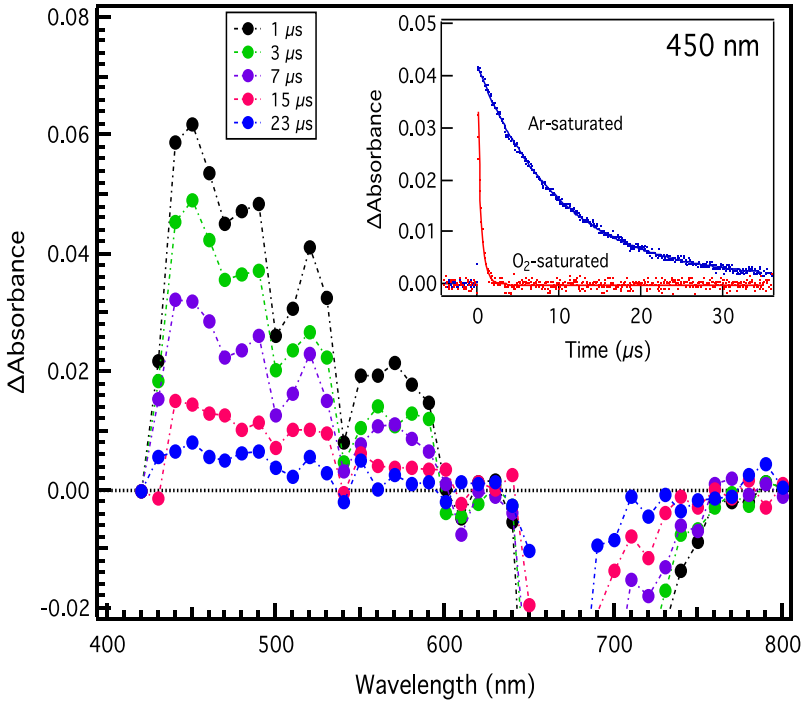



**Figure S20.** Nanosecond transient absorption spectra at the indicated time intervals of the **5** in Ar-saturated toluene solution. Inset shows the decay profile of the triplet state of **5** in Ar-saturated and oxygen-saturated solutions.

## Molecular Formula Strings



| | |
|---|---|
| 1 | C[C@@H]([C@@H]/1CCC(OC)=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC(I)=C3)C2=C\C4=N/C(C(CC)=C4C)=C\5)=NC1=C(CC6=O)/C7=C6C(C)=C5N7 |
| 2 | C[C@@H]([C@@H]/1CCC(OC)=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC([I124])=C3)C2=C\C4=N/C(C(CC)=C4C)=C\5)=NC1=C(CC6=O)/C7=C6C(C)=C5N7 |
| 3 | C[C@@H]([C@@H]/1CCC(NCC2=CC(I)=CC=C2)=O)C(/C=C(N/3)/C(C)=C(C(C)OCC4=CC=CC(C#CC5=CC(NC6=C(C=C(OCCOC)C(OCCOC)=C7)C7=NC=N6)=CC=C5)=C4)C3=C\C8=N/C(C(CC)=C8C)=C\9)=NC1=C(CC%10=O)/C%11=C%10C(C)=C9N%11 |
| 4 | C[C@@H]([C@@H]/1CCC(NCC2=CC([I124])=CC=C2)=O)C(/C=C(N/3)/C(C)=C(C(C)OCC4=CC=CC(C#CC5=CC(NC6=C(C=C(OCCOC)C(OCCOC)=C7)C7=NC=N6)=CC=C5)=C4)C3=C\C8=N/C(C(CC)=C8C)=C\9)=NC1=C(CC%10=O)/C%11=C%10C(C)=C9N%11 |
| 5 | C[C@@H]([C@@H]/1CCC([NH])=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC(I)=C3)C2=C\C4=N/C(C(CC)=C4C)=C\5)=NC1=C(CC6=O)/C7=C6C(C)=C5N7.COCCOC(C(OCCOC)=C8)=CC(C8=NC=N9)=C9NC%10=CC=CC(C#CC%11=CC(CC)=CC=C%11)=C%10 |
| 6 | C[C@@H]([C@@H]/1CCC([NH])=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC([I124])=C3)C2=C\C4=N/C(C(CC)=C4C)=C\5)=NC1=C(CC6=O)/C7=C6C(C)=C5N7.COCCOC(C(OCCOC)=C8)=CC(C8=NC=N9)=C9NC%10=CC=CC(C#CC%11=CC(CC)=CC=C%11)=C%10 |
| 7 | C#CC1=CC(NC2=C(C=C(OCCOC)C(OCCOC)=C3)C3=NC=N2)=CC=C1 |
| 8 | C[C@@H]([C@@H]/1CCC(OC)=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC(C#CC4=CC(NC5=C(C=C(OCCOC)C(OCCOC)=C6)C6=NC=N5)=CC=C4)=C3)C2=C\C7=N/C(C(CC)=C7C)=C\8)=NC1=C(CC9=O)/C%10=C9C(C)=C8N%10 |
| 9 | C[C@@H]([C@@H]/1CCC(O)=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC(C#CC4=CC(NC5=C(C=C(OCCOC)C(OCCOC)=C6)C6=NC=N5)=CC=C4)=C3)C2=C\C7=N/C(C(CC)=C7C)=C\8)=NC1=C(CC9=O)/C%10=C9C(C)=C8N%10 |
| 10 | C[C@@H]([C@@H]/1CCC(NCC2=CC([Sn](C)(C)C)=CC=C2)=O)C(/C=C(N/3)/C(C)=C(C(C)OCC4=CC=CC(C#CC5=CC(NC6=C(C=C(OCCOC)C(OCCOC)=C7)C7=NC=N6)=CC=C5)=C4)C3=C\C8=N/C(C(CC)=C8C)=C\9)=NC1=C(CC%10=O)/C%11=C%10C(C)=C9N%11 |
| 11 | NCC1=CC=CC(C#CC2=CC(NC3=C(C=C(OCCOC)C(OCCOC)=C4)C4=NC=N3)=CC=C2)=C1 |
| 12 | C[C@@H]([C@@H]/1CCC(O)=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC(I)=C3)C2=C\C4=N/C(C(CC)=C4C)=C\5)=NC1=C(CC6=O)/C7=C6C(C)=C5N7 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 13 | C[C@@H]([C@@H]/1CCC([NH])=O)C(/C=C(N/2)/C(C)=C(C(C)OCC3=CC=CC([Sn](C)(C)C)=C3)C2=C\C4=N/C(C(CC)=C4C)=C\5)=NC1=C(CC6=O)/C7=C6C(C)=C5N7.COCCOC(C(OCCOC)=C8)=CC(C8=NC=N9)=C9NC%10=CC=CC(C#CC%11=CC(CC)=CC=C%11)=C%10 | | | | | | | | | | | | | | | | | | | | | | |
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