

Supplementary Information

Photovoltaic performances of type-II dye-sensitized solar cells based on catechol dye sensitizers: retardation of back-electron transfer by PET (photo-induced electron transfer)

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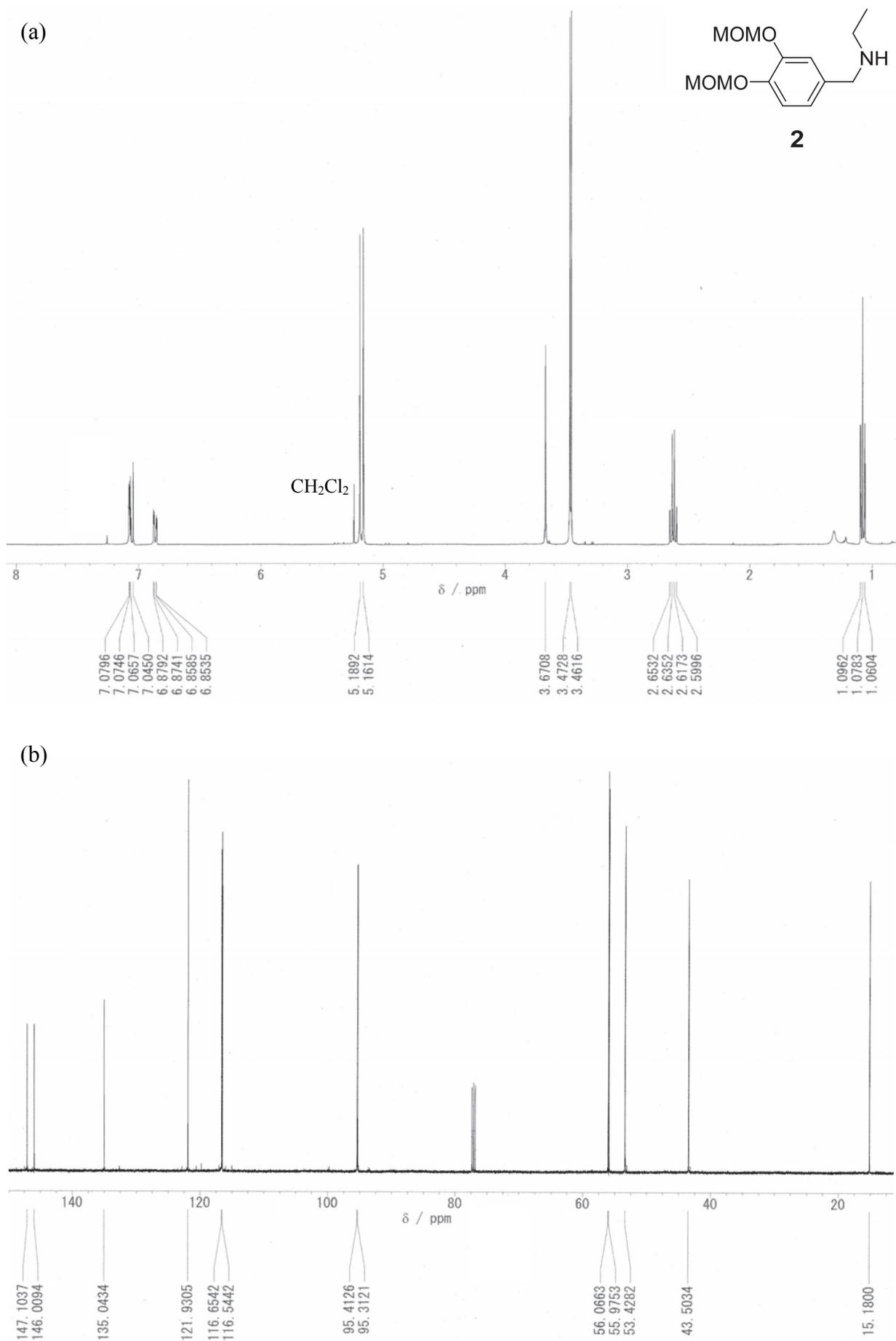


Fig. S1 (a) ¹H NMR (400 MHz) and (b) ¹³C NMR (125 MHz) of **2** in CDCl₃.

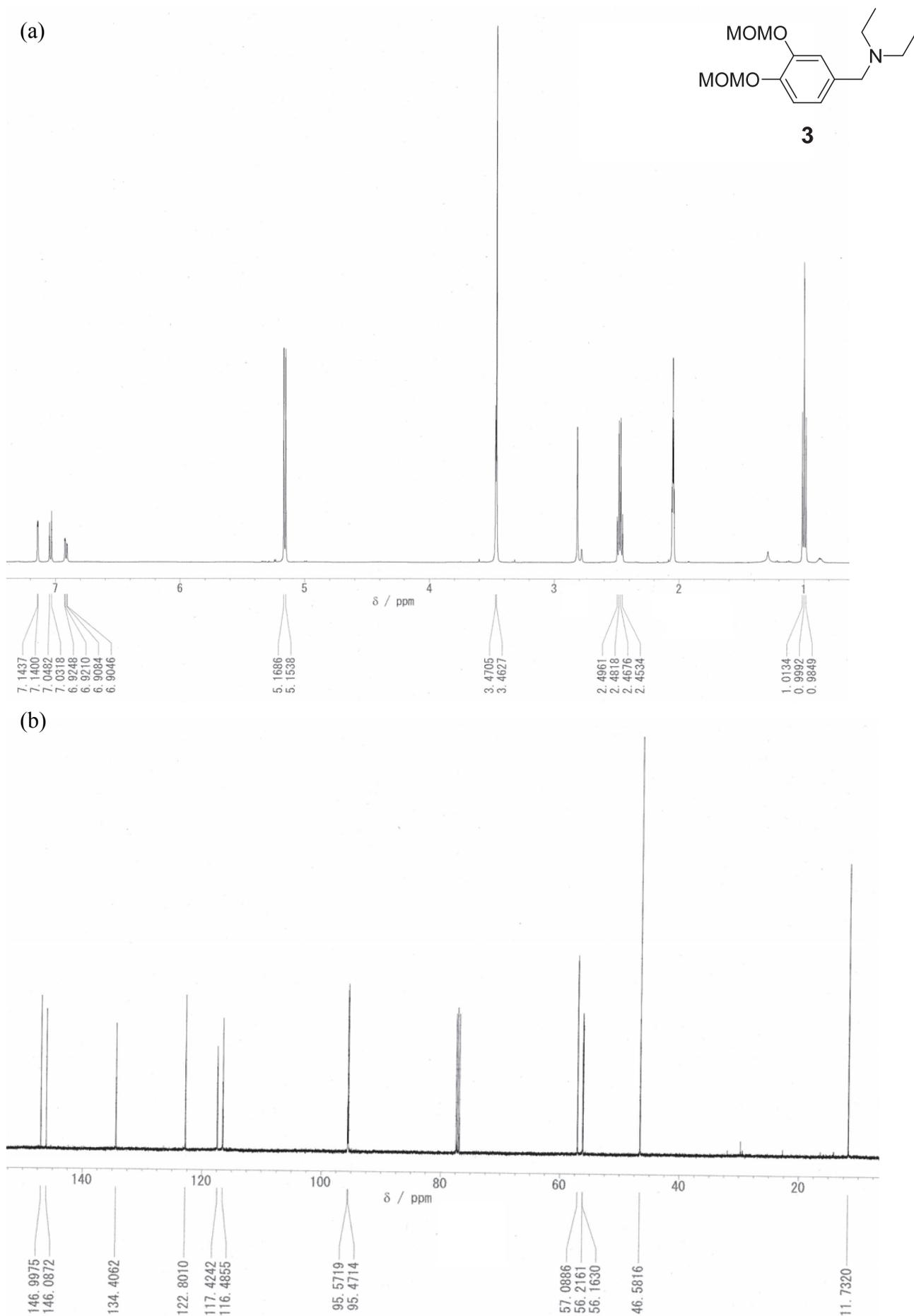
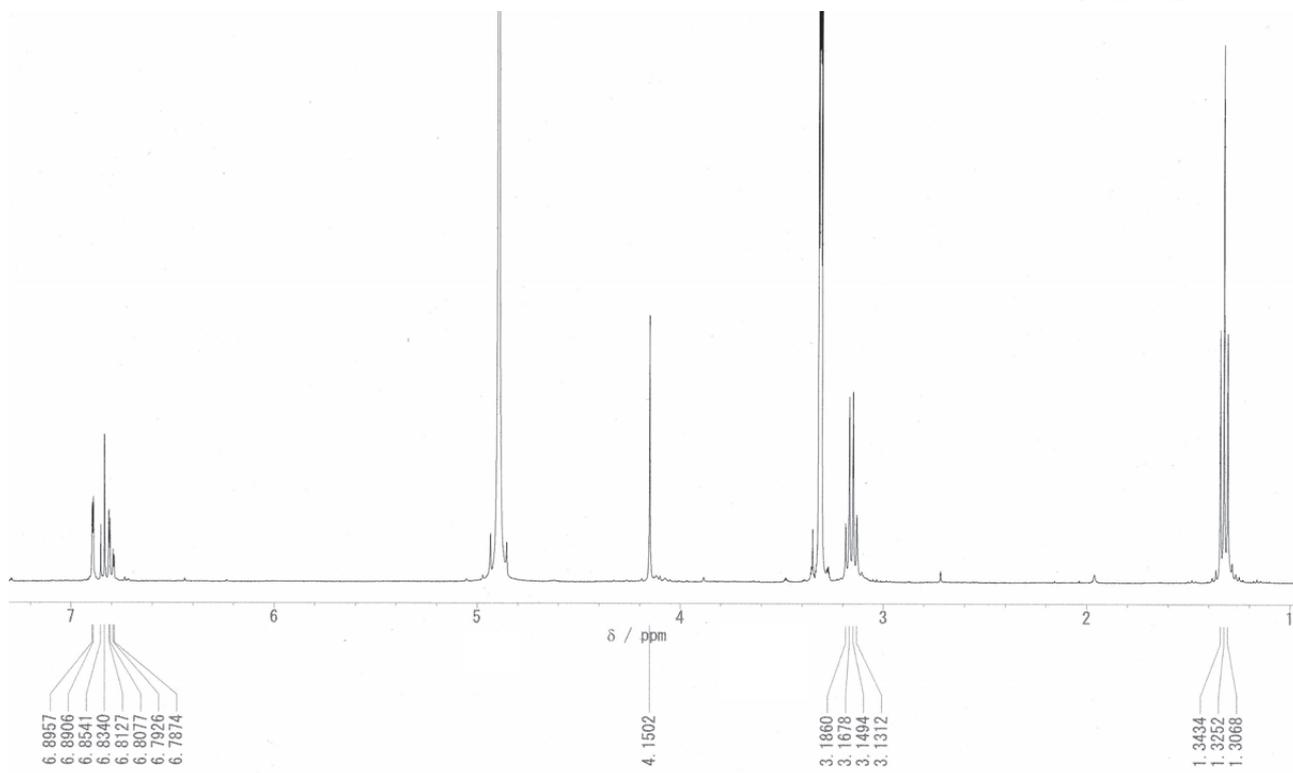
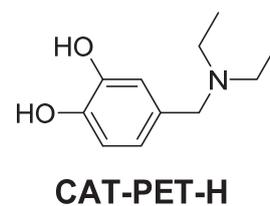


Fig. S2 (a) ^1H NMR (500 MHz) of **3** in acetone- d_6 and (b) ^{13}C NMR (125 MHz) of **3** in CDCl_3 .

(a)



(b)

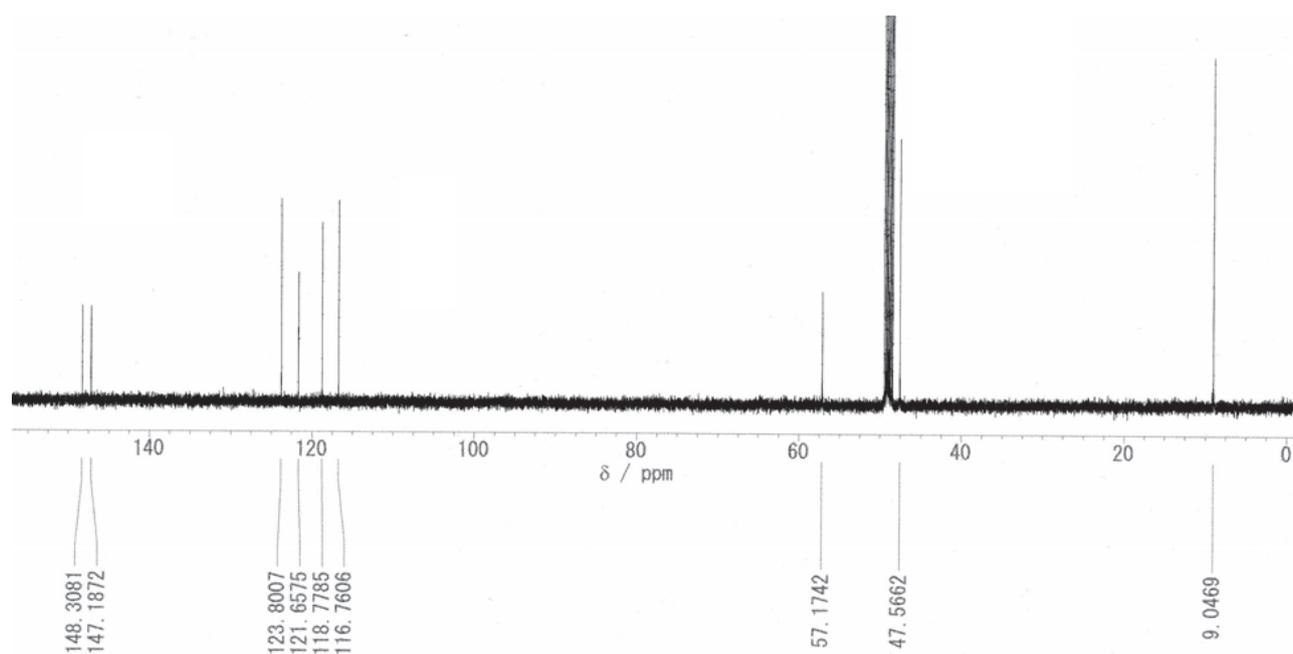


Fig. S3 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) of **CAT-PET-H** in CD_3OD .

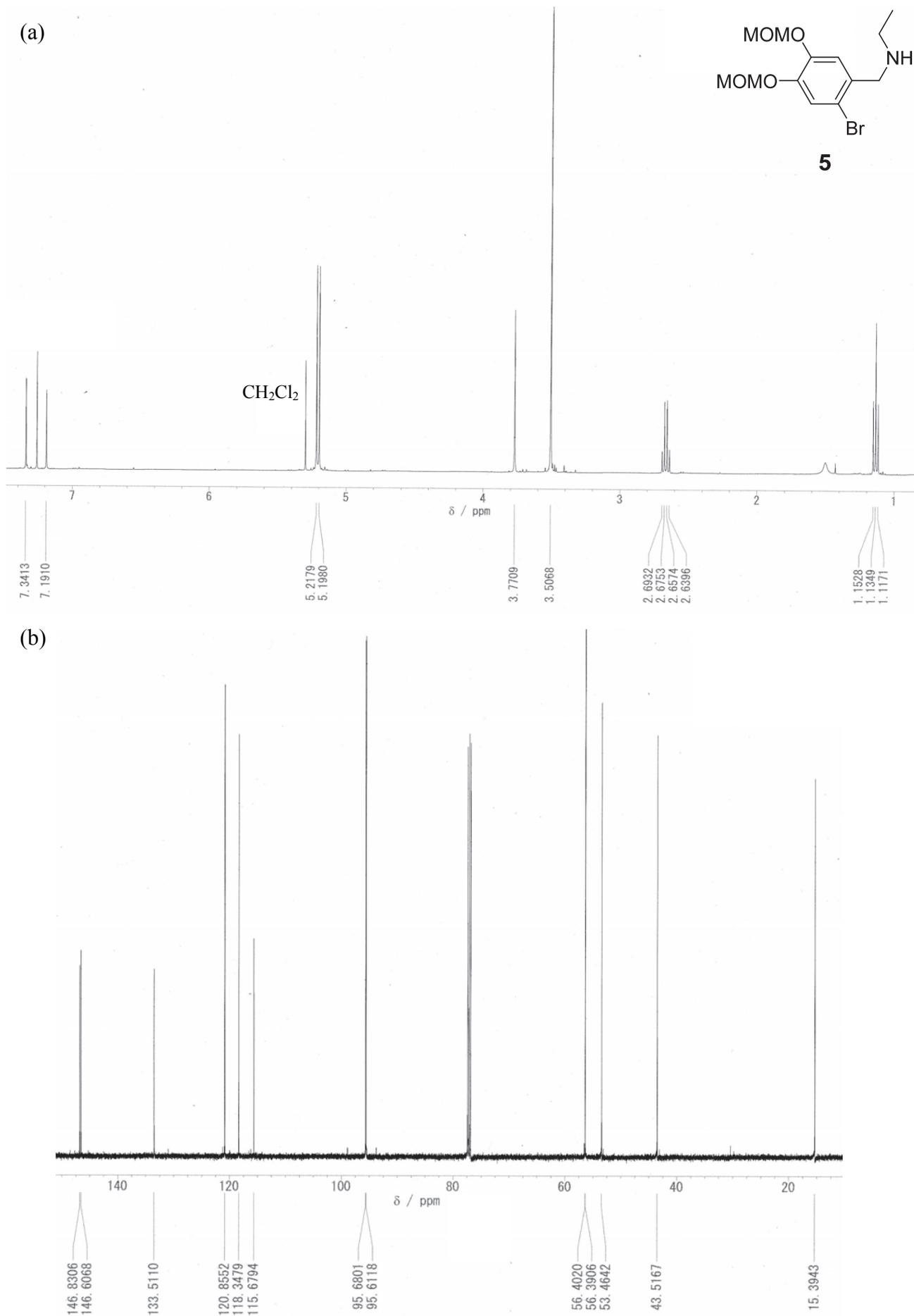


Fig. S4 (a) ¹H NMR (400 MHz) and (b) ¹³C NMR (125 MHz) of **5** in CDCl₃.

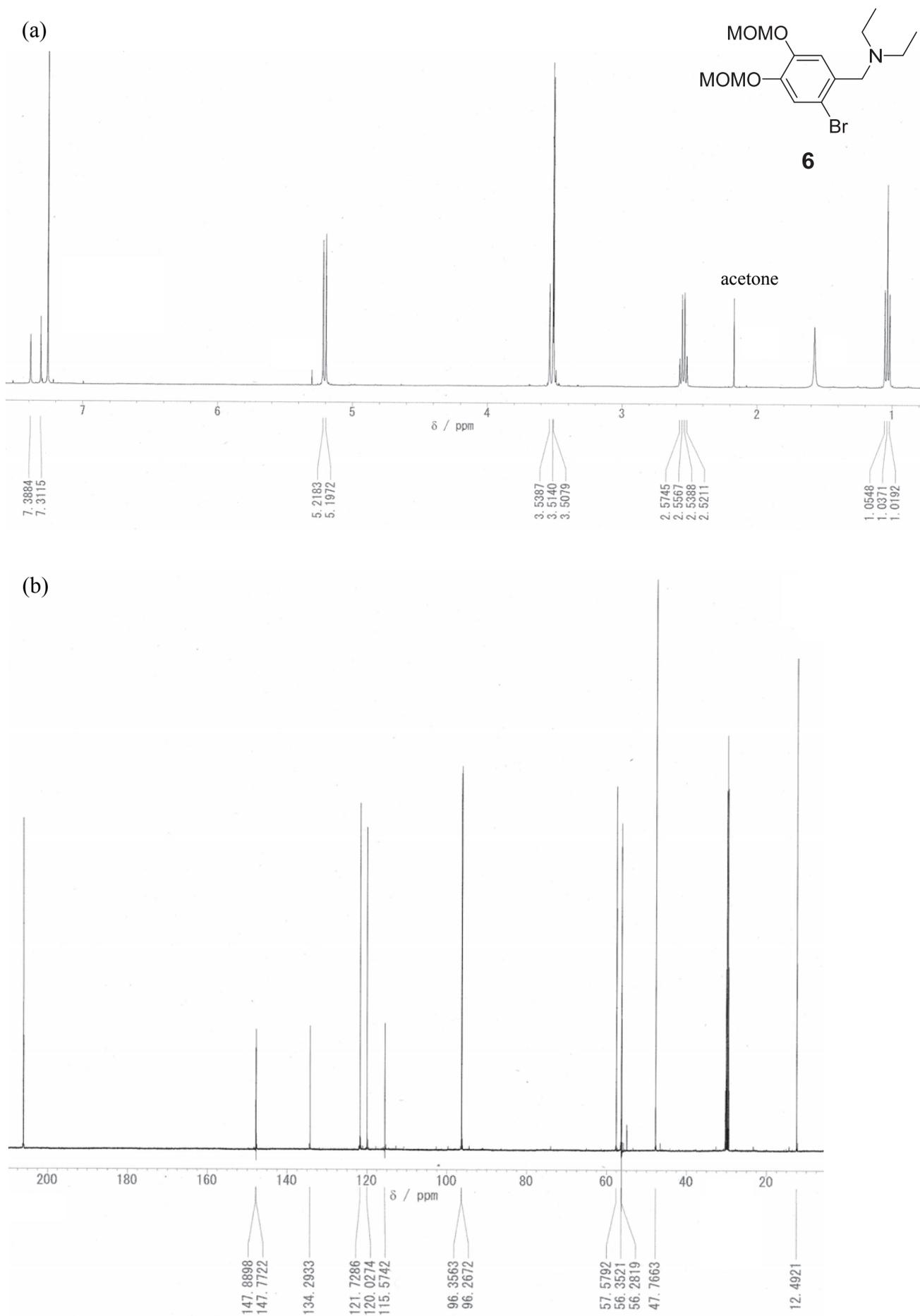
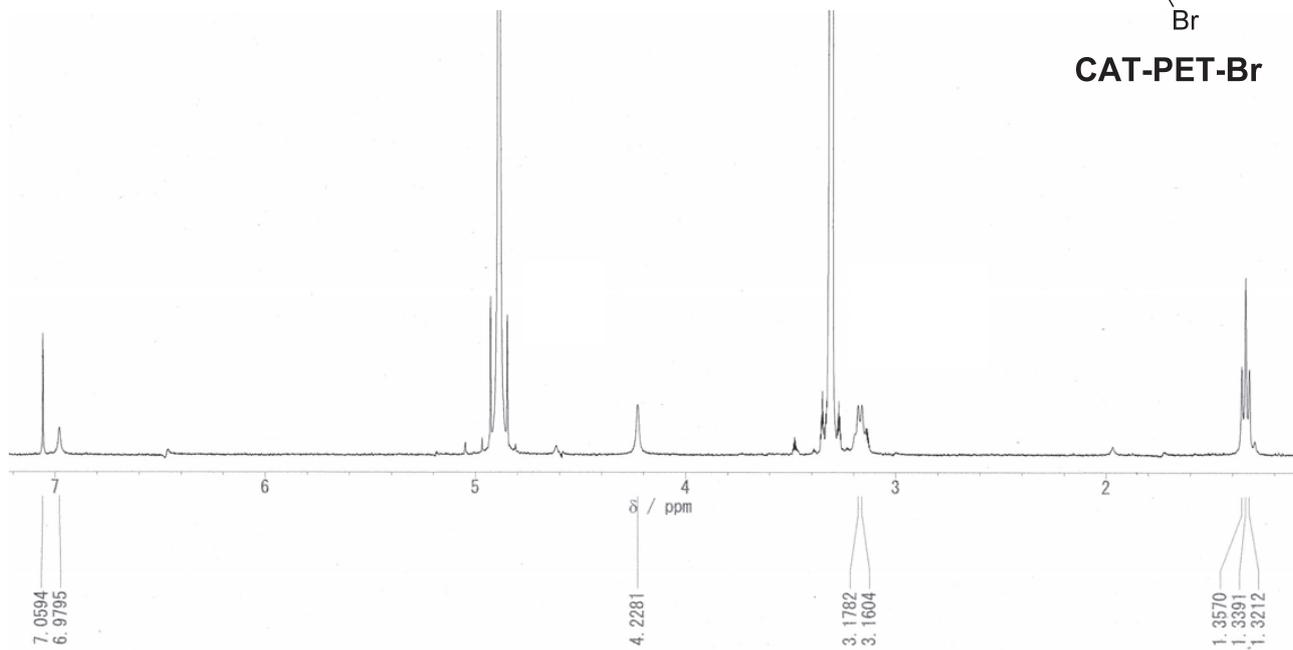
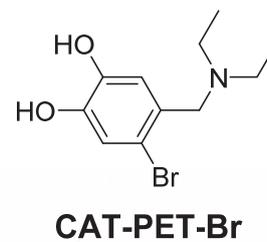


Fig. S5 (a) ^1H NMR (400 MHz) of **6** in CDCl_3 and (b) ^{13}C NMR (125 MHz) of **6** in acetone-d_6 .

(a)



(b)

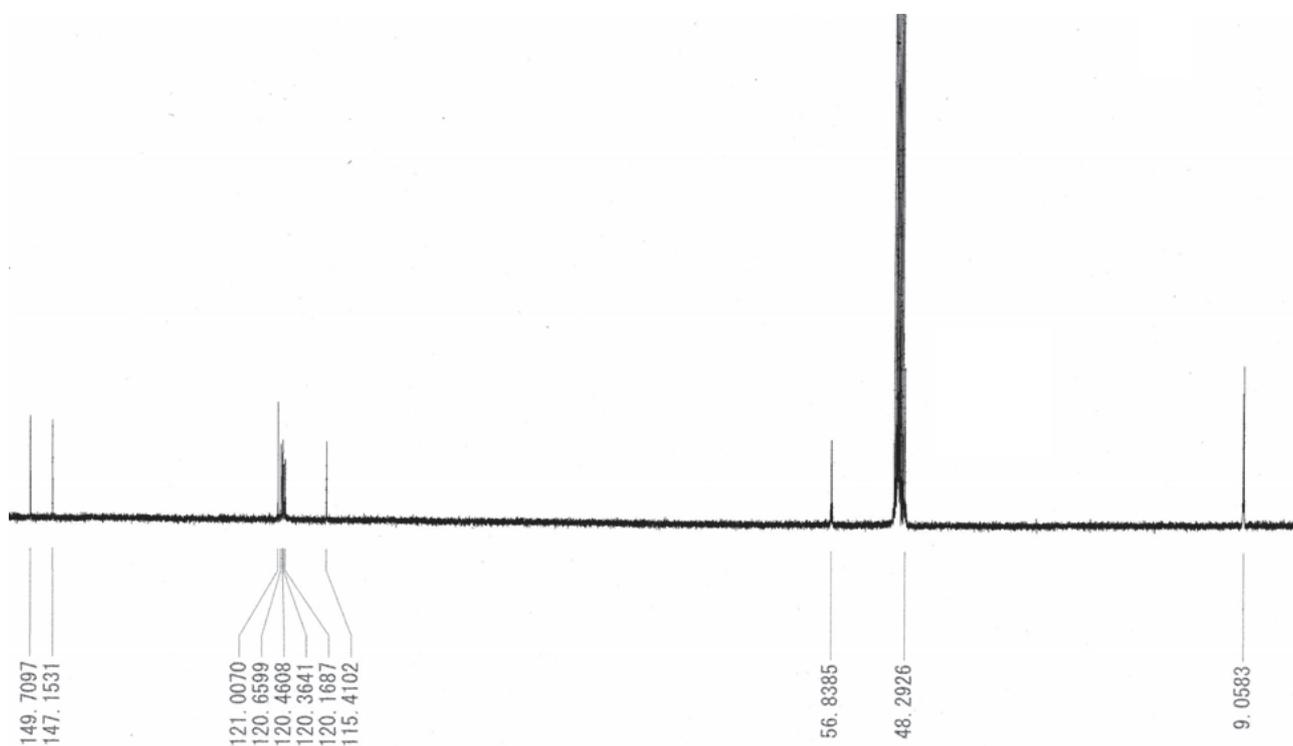
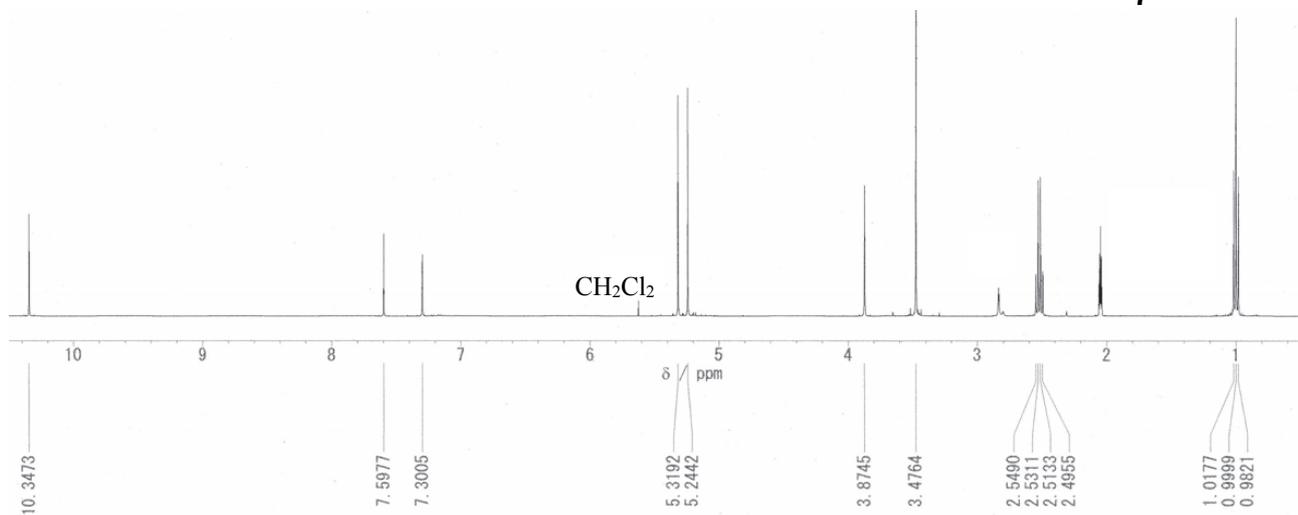
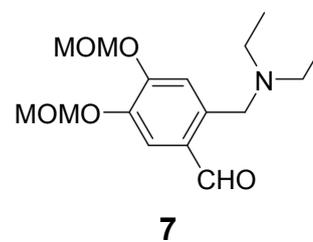


Fig. S6 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) of **CAT-PET-Br** in CD_3OD .

(a)



(b)

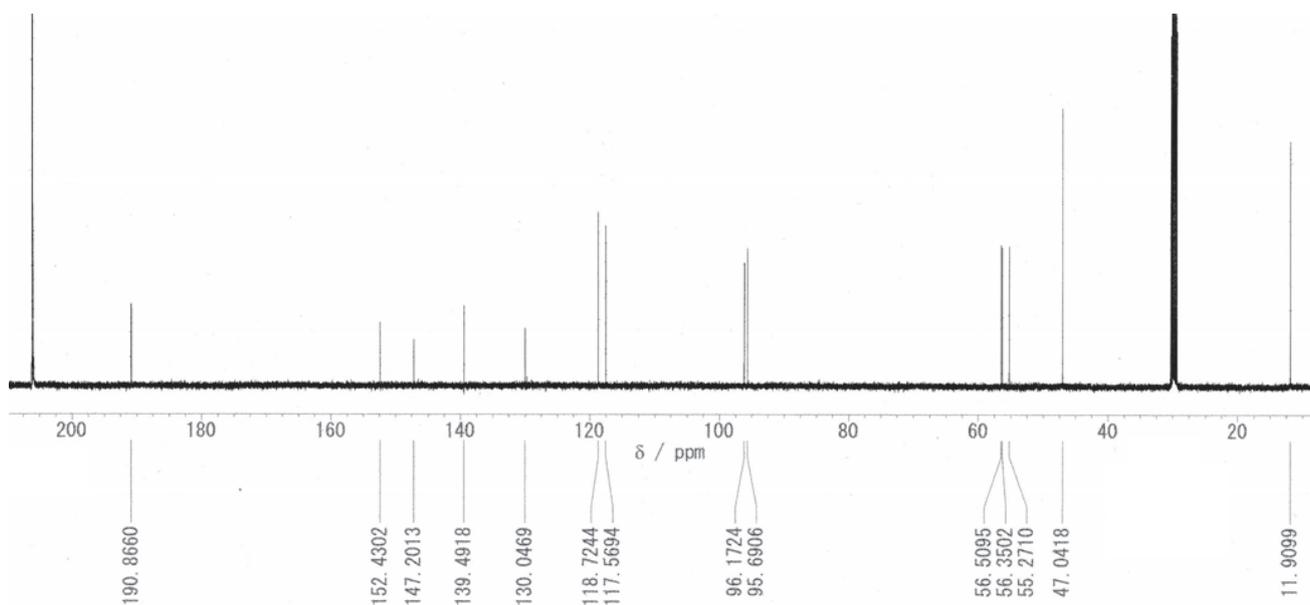
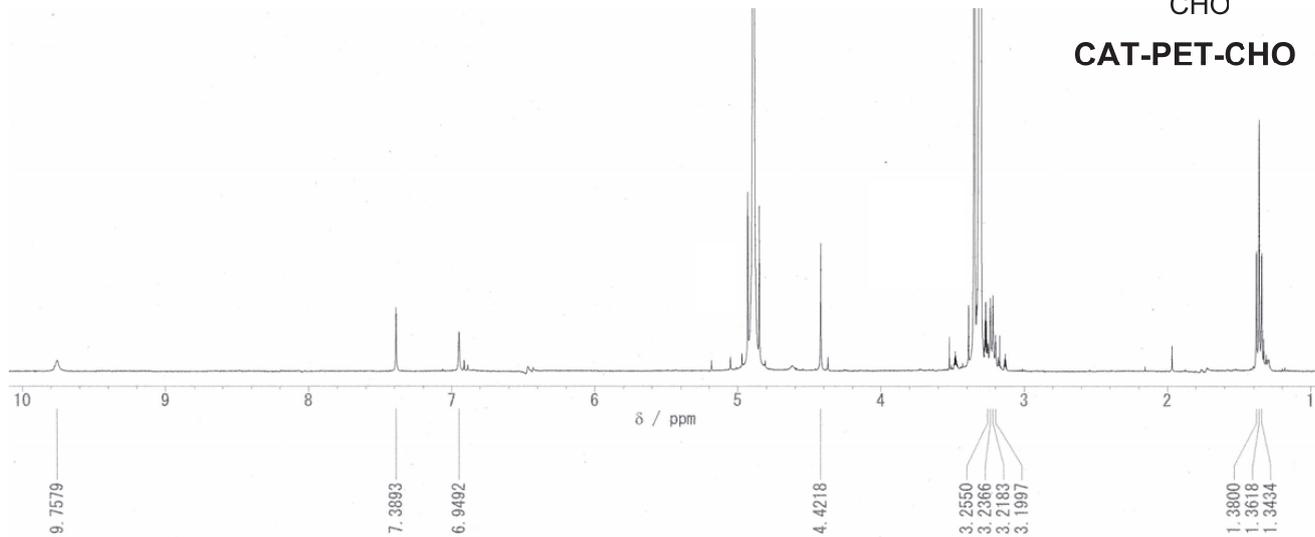
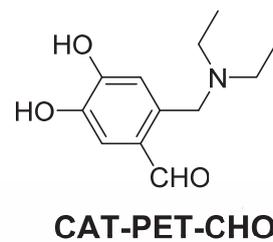


Fig. S7 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) of **7** in acetone- d_6 .

(a)



(b)

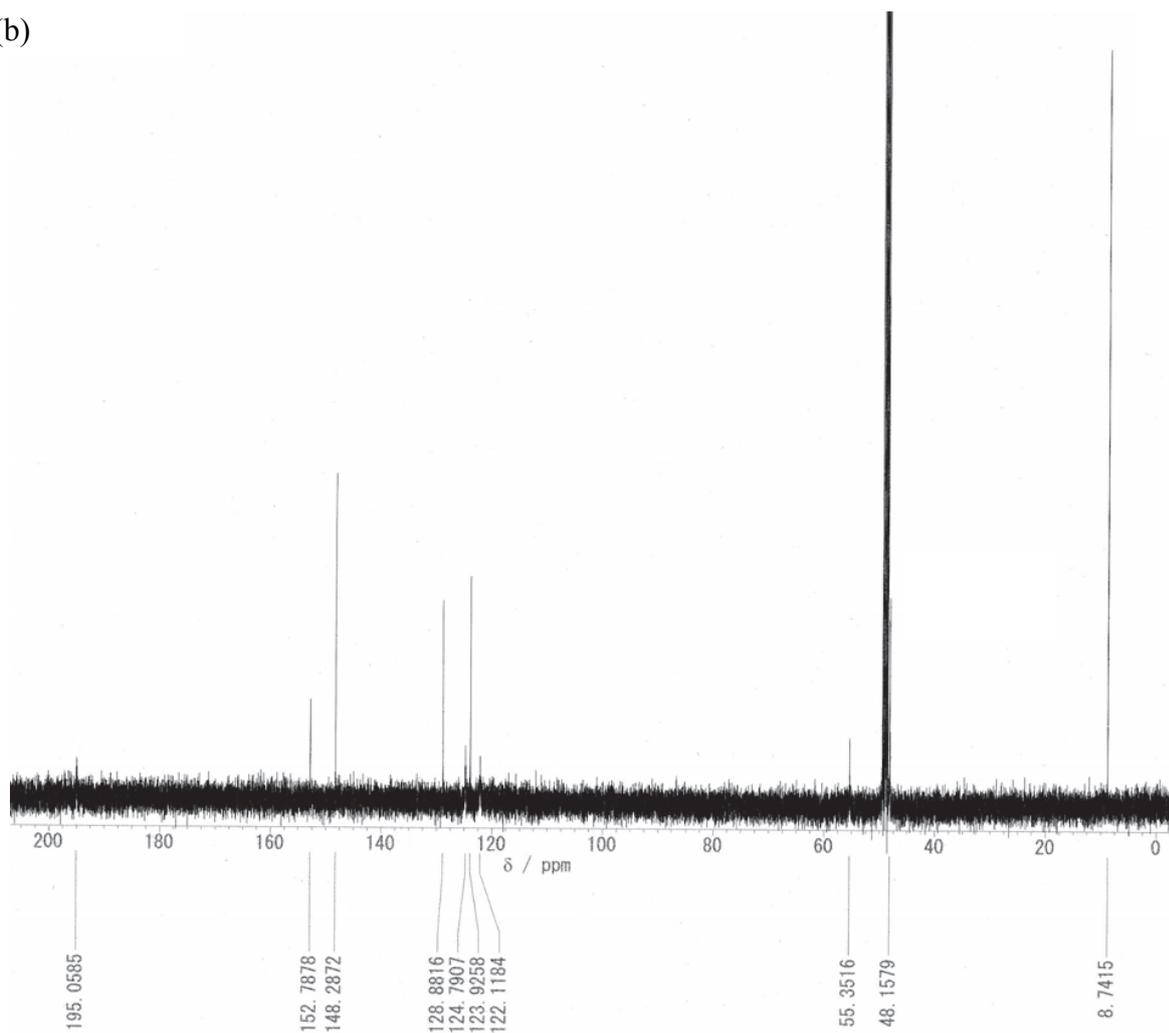


Fig. S8 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) of **CAT-PET-CHO** in CD_3OD .

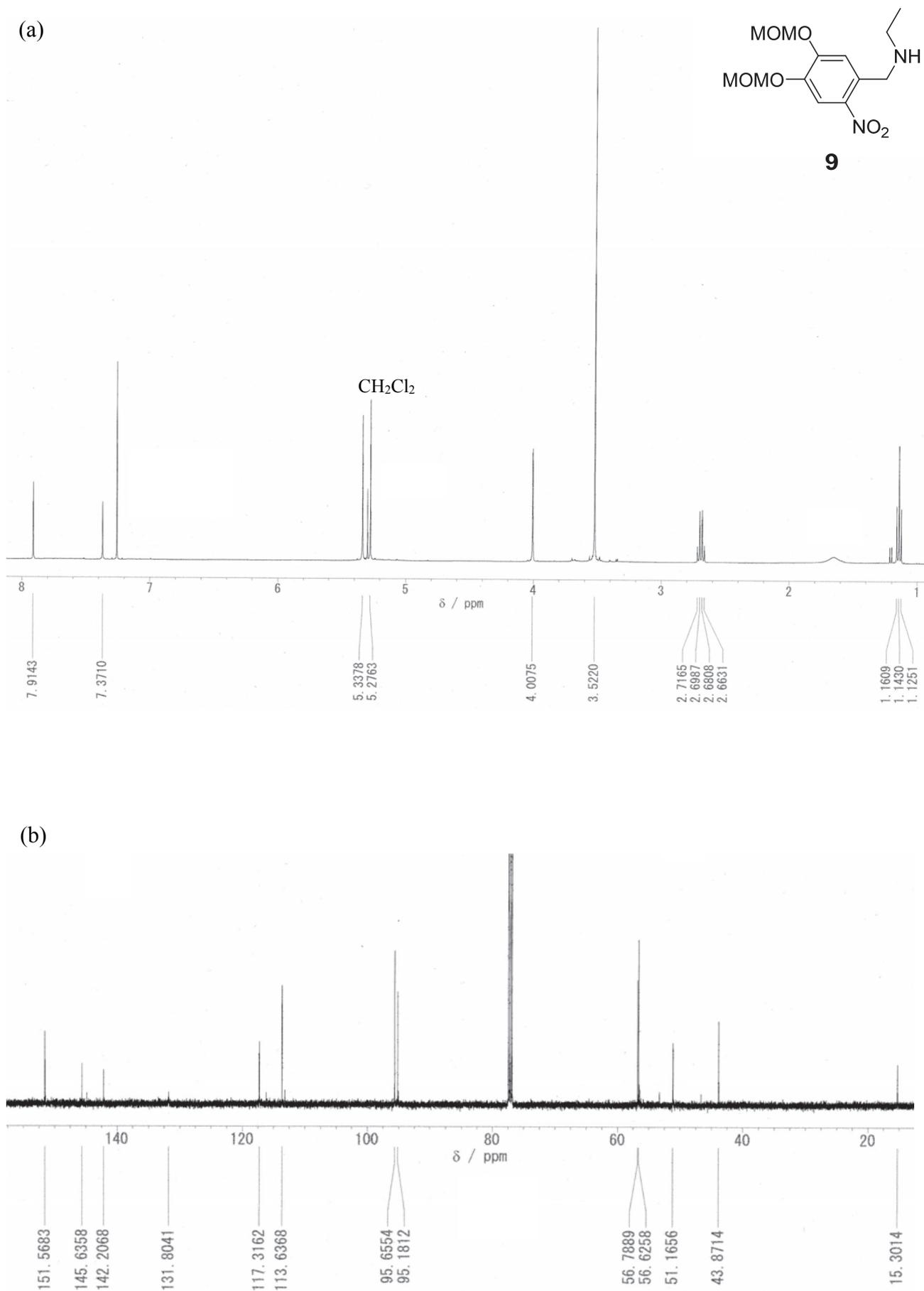
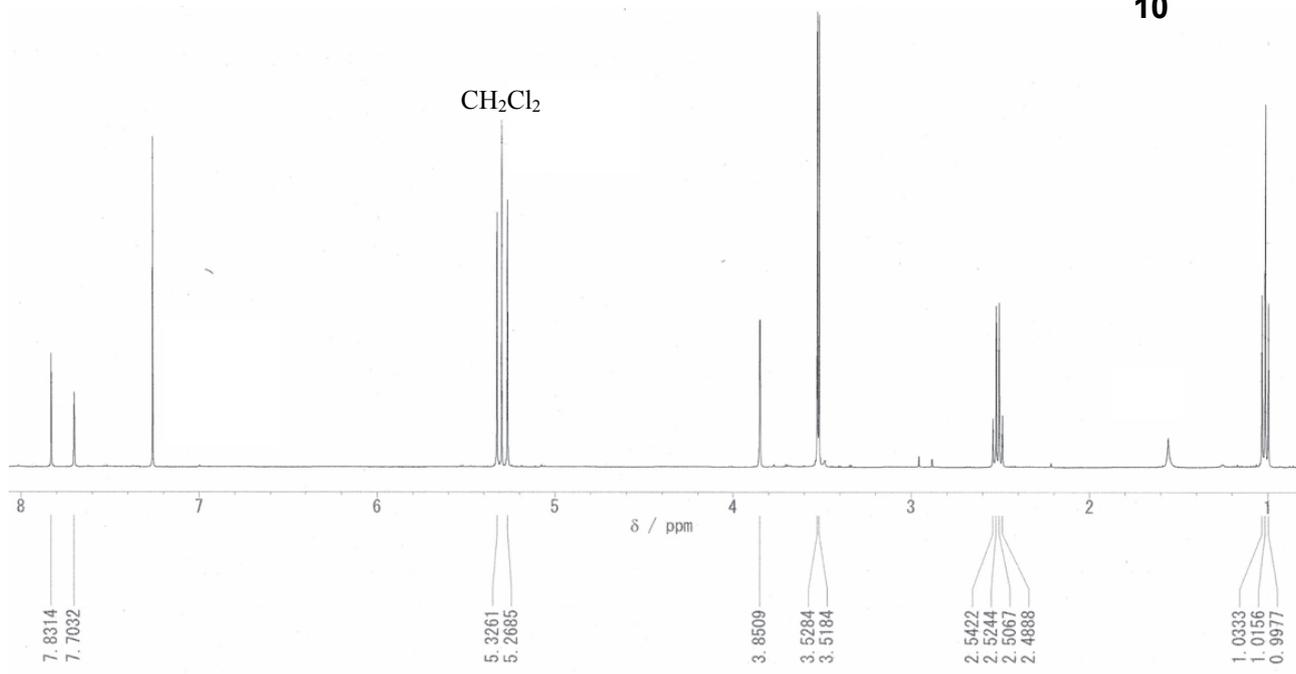
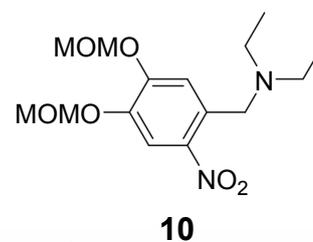


Fig. S9 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) of **9** in CDCl_3 .

(a)



(b)

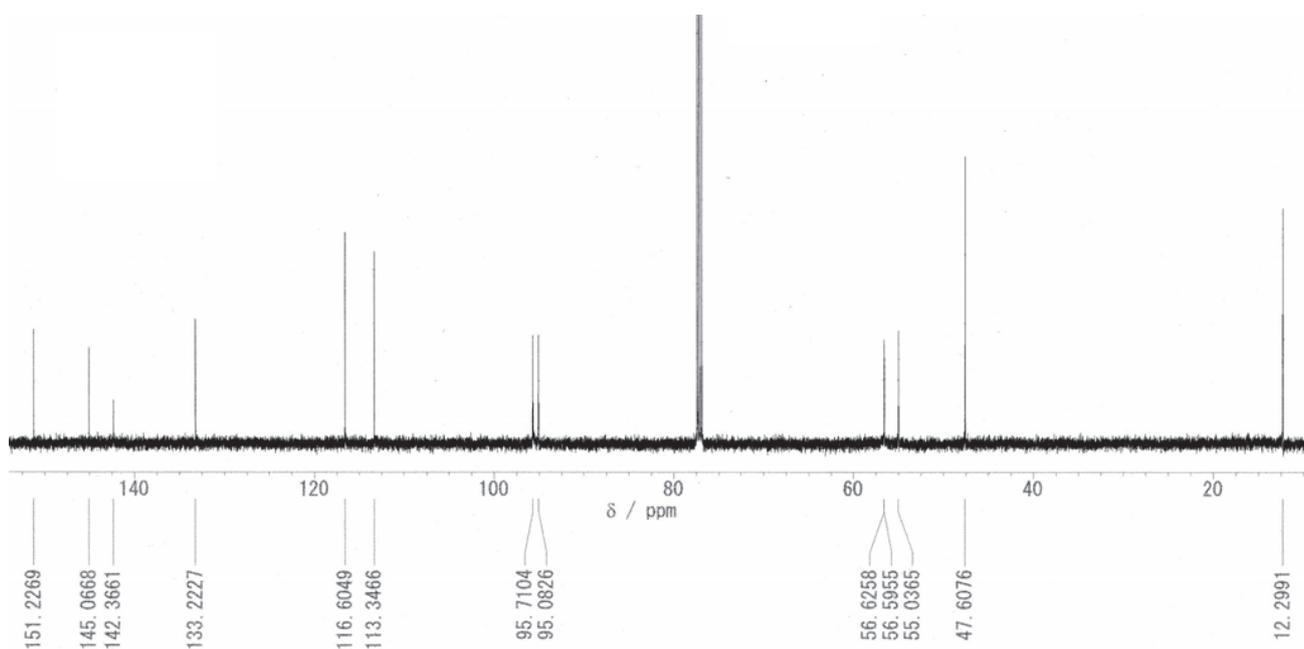
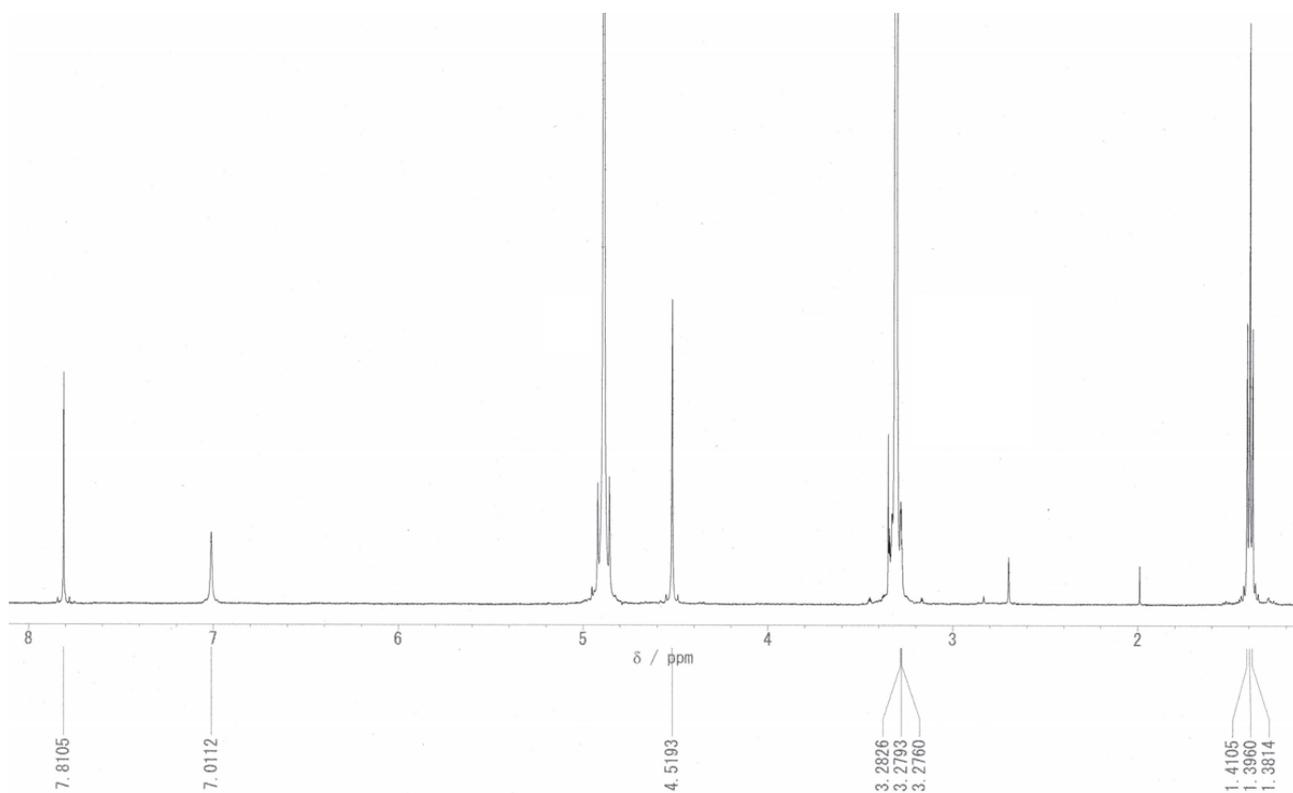
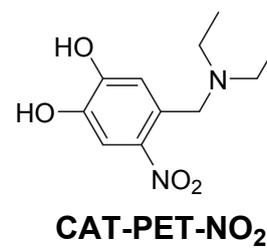


Fig. S10 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) of **10** in CDCl_3 .

(a)



(b)

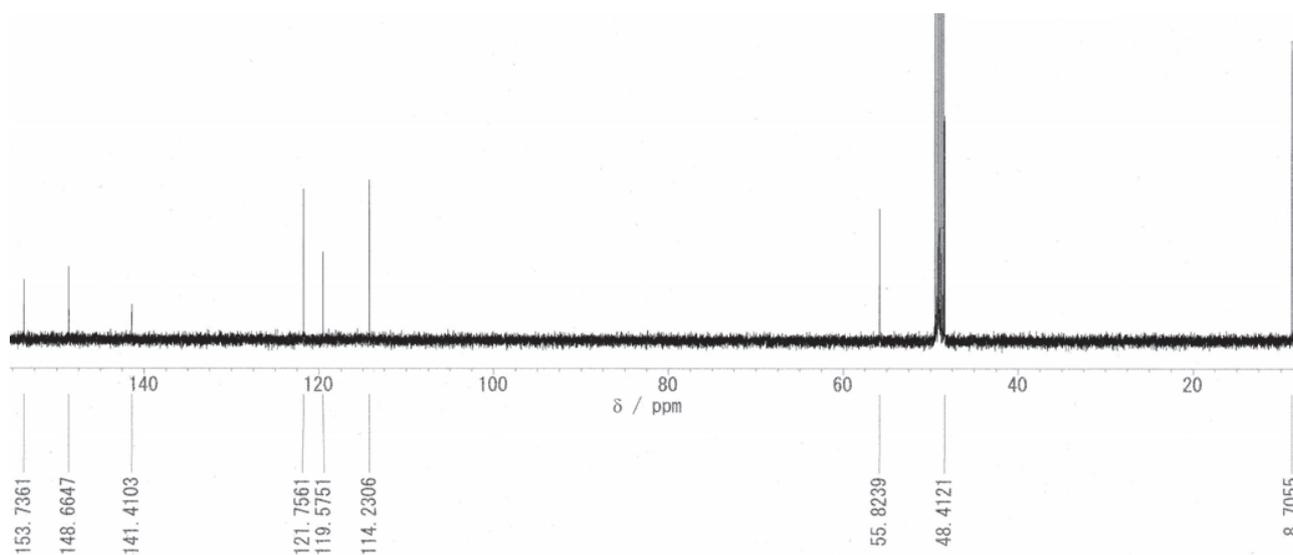


Fig. S11 (a) ¹H NMR (500 MHz) and (b) ¹³C NMR (125 MHz) of **CAT-PET-NO₂** in CD₃OD.

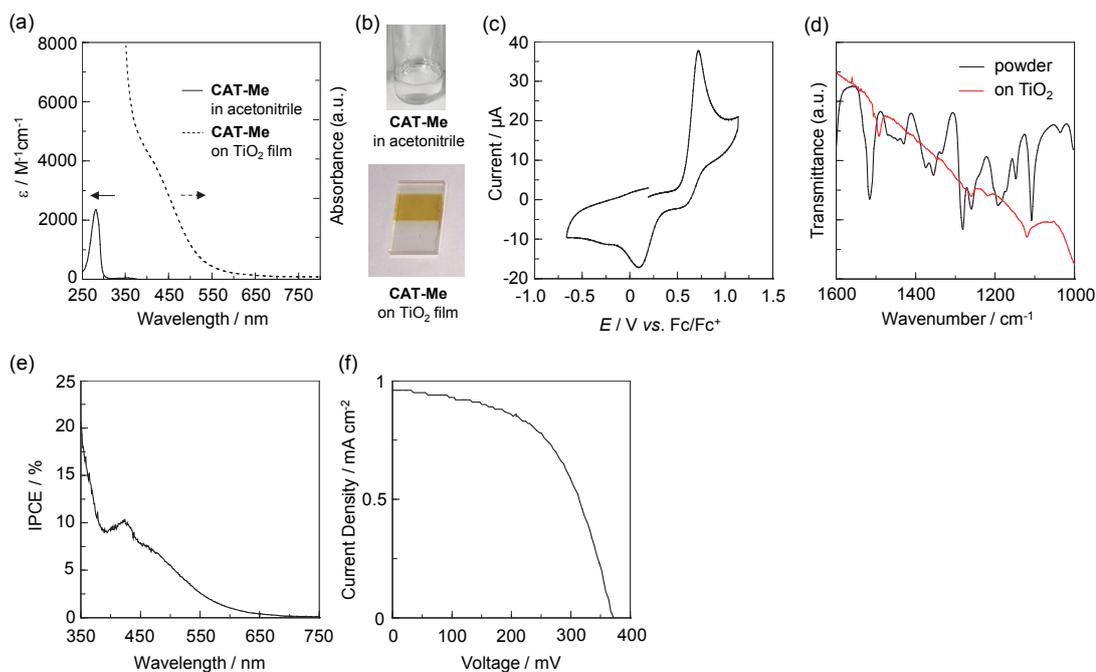


Fig. S12 (a) Photoabsorption spectra and (b) photographs of **CAT-Me** in acetonitrile and adsorbed on TiO₂ film. (c) Cyclic voltammogram of **CAT-Me** in acetonitrile containing 0.1 M Bu₄NClO₄. (d) FTIR spectra of the powders and the dyes adsorbed on TiO₂ nanoparticles for **CAT-Me**. (e) IPCE spectrum and (f) $I-V$ curve of DSSC based on **CAT-Me**.

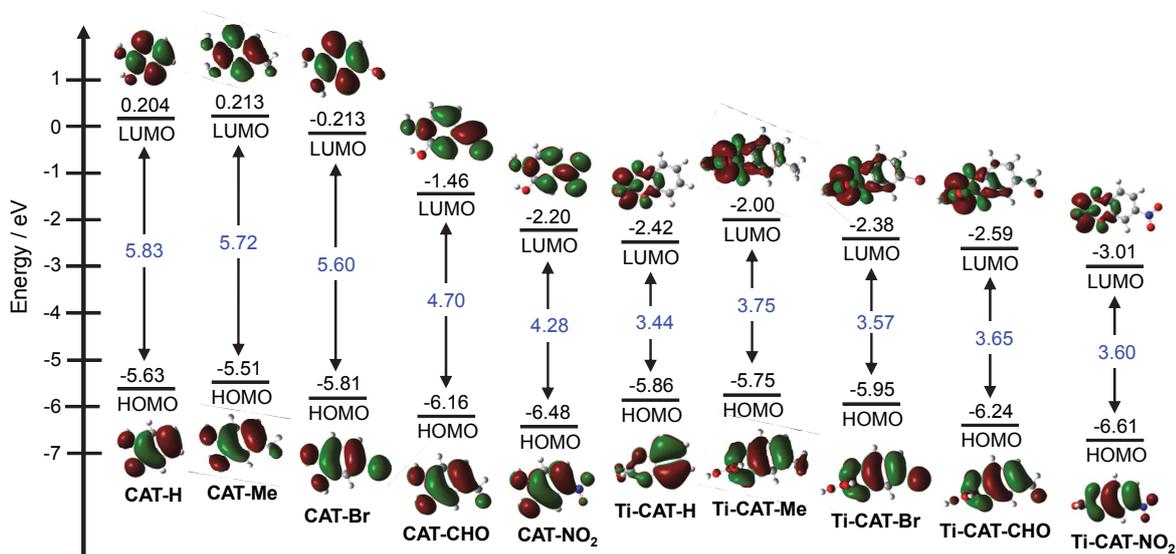


Fig. S13 Energy level diagram, HOMO and LUMO of CAT dyes and their Ti-complexes (**Ti-CAT**), derived from DFT calculations.