

Supplementary File

Indole-3-carboxamido-Polyamine Conjugates Target Bacterial Membranes and are Antimicrobial and Antibiotic Potentiators

Kenneth Sue ¹, Melissa M. Cadelis ^{1,2}, Florent Rouvier ³, Marie-Lise Bourguet-Kondracki ⁴, Jean Michel Brunel ³ and Brent R. Copp ^{1,*}

¹ School of Chemical Sciences, The University of Auckland, Private Bag 92019, Auckland 1142, New Zealand

² School of Medical Sciences, The University of Auckland, Private Bag 92019, Auckland 1142, New Zealand

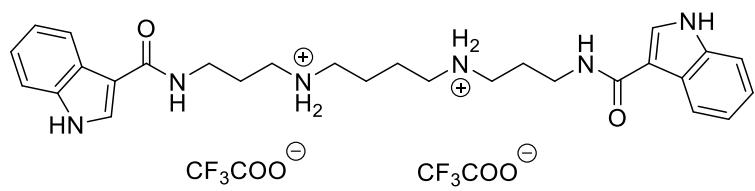
³ Membranes et Cibles Thérapeutiques, INSERM, Aix-Marseille Université, 27 bd Jean Moulin, 13385 Marseille, France

⁴ Laboratoire Molécules de Communication et Adaptation des Micro-organismes, UMR 7245 CNRS, Muséum National d'Histoire Naturelle, 57 rue Cuvier (C.P. 54), 75005 Paris, France

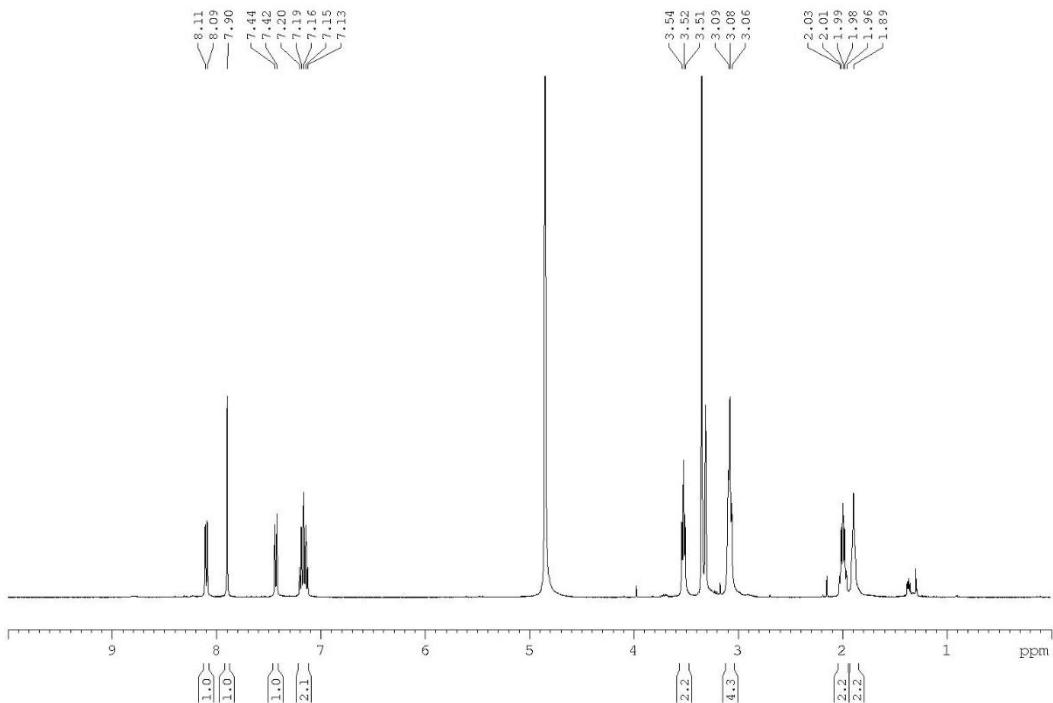
* Correspondence: b.copp@auckland.ac.nz

Contents

Figure S1 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 12a	S3
Figure S2 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 12b	S4
Figure S3 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 12c	S5
Figure S4 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 12d	S6
Figure S5 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 12e	S7
Figure S6 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 12f	S8
Figure S7 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 13b	S9
Figure S8 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 13c	S10
Figure S9 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 13d	S11
Figure S10 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 13e	S12
Figure S11 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 13f	S13
Figure S12 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 14a	S14
Figure S13 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 14b	S15
Figure S14 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 14c	S16
Figure S15 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 14d	S17
Figure S16 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 14e	S18
Figure S17 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 14f	S19
Figure S18 ¹ H (CD ₃ OD, 400 MHz) and ¹³ C (CD ₃ OD, 100 MHz) NMR spectra for 15a	S20



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

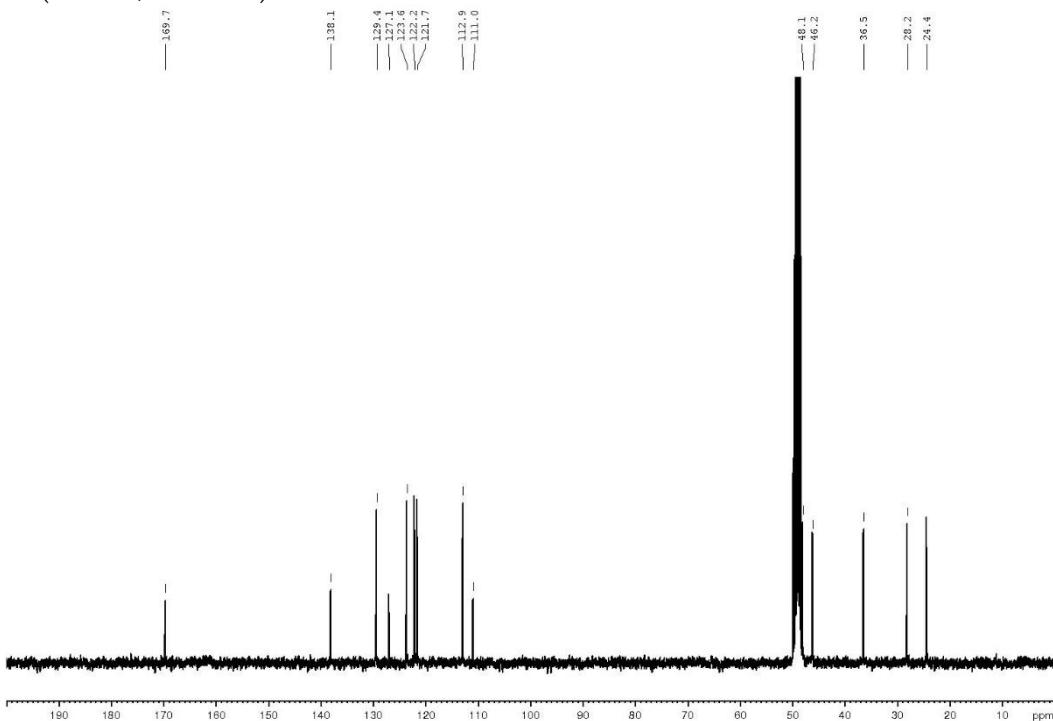
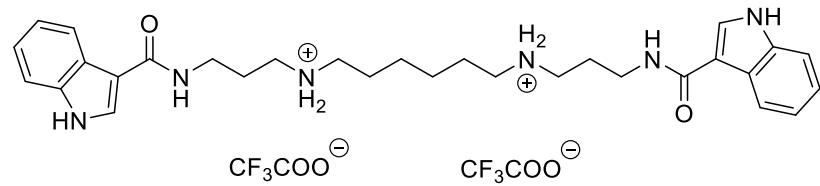
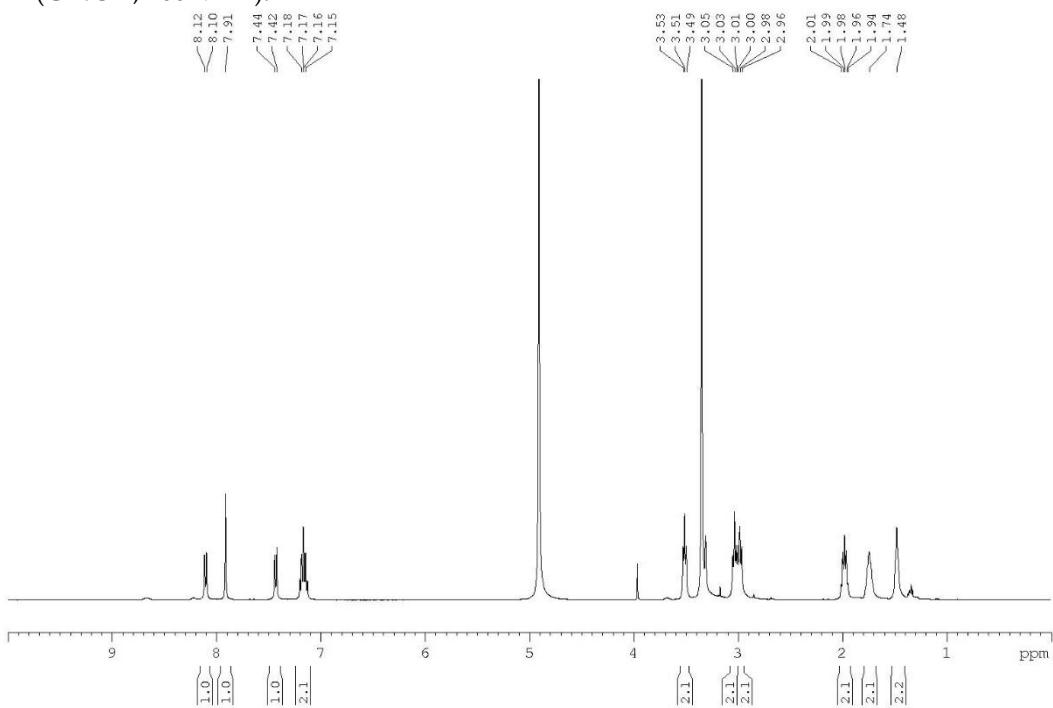


Figure S1 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **12a**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

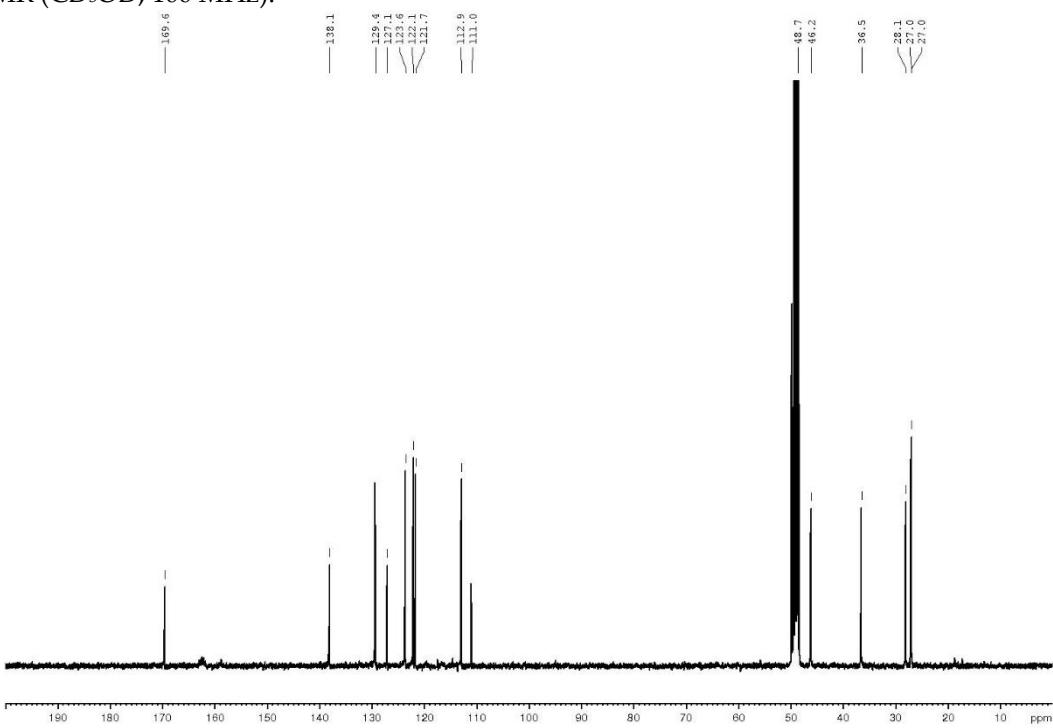
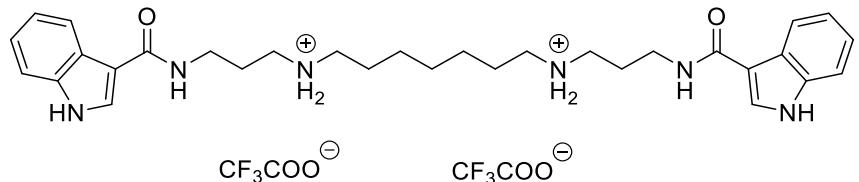
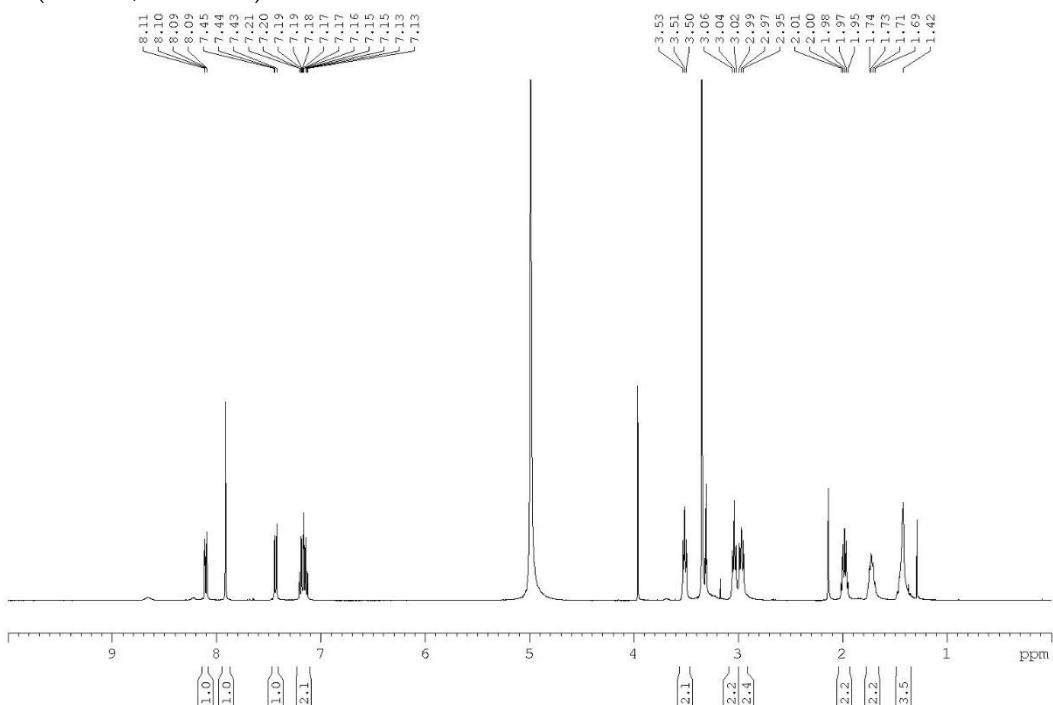


Figure S2 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **12b**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

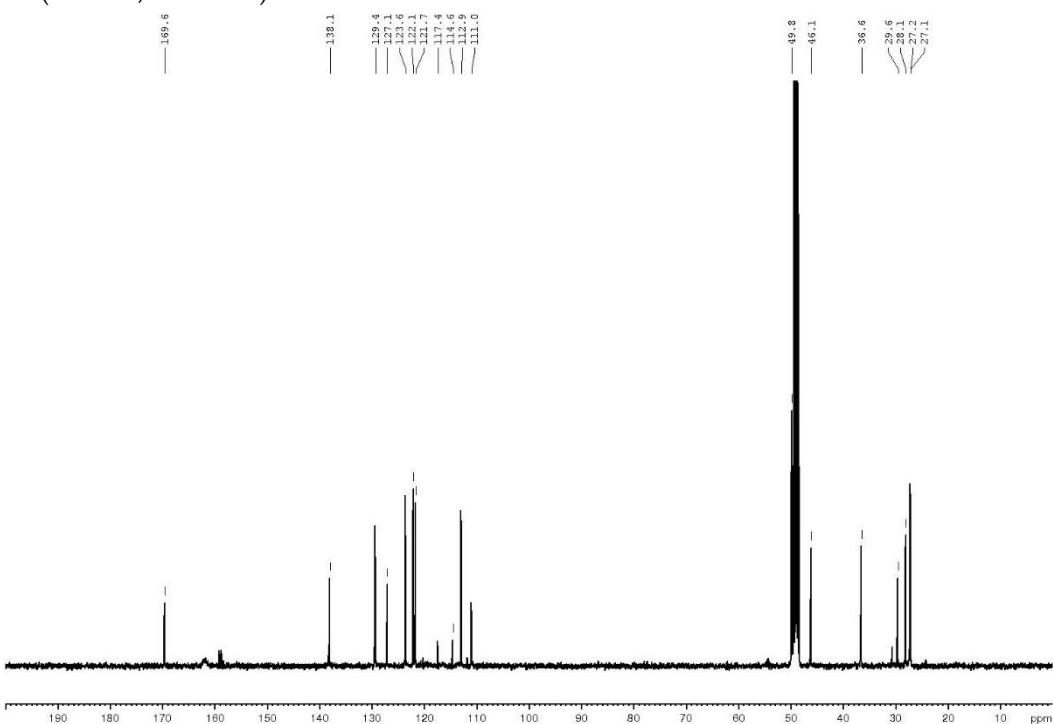
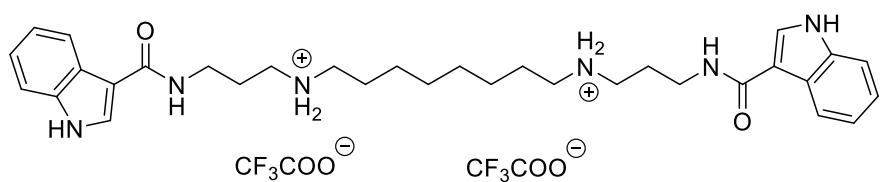
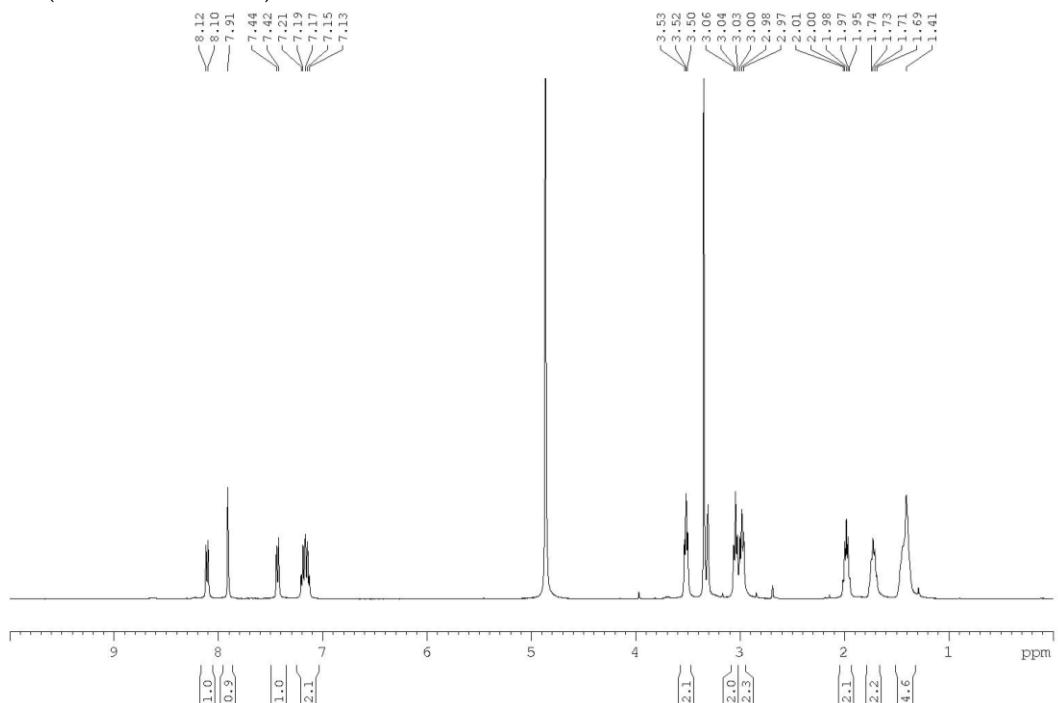


Figure S3 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **12c**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

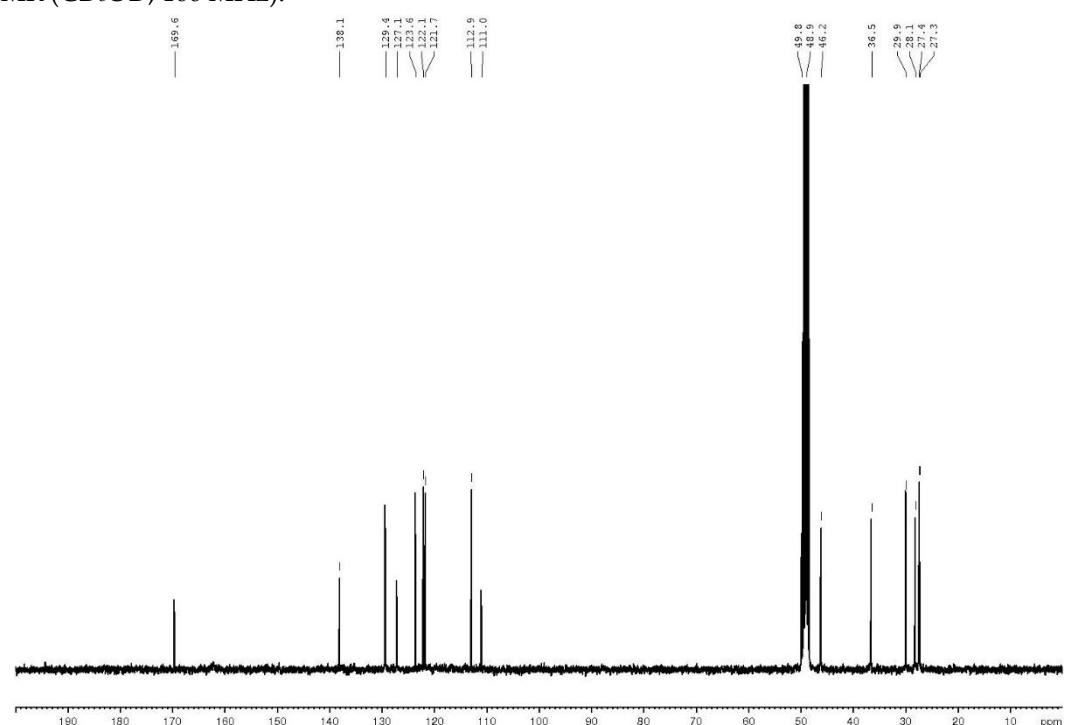
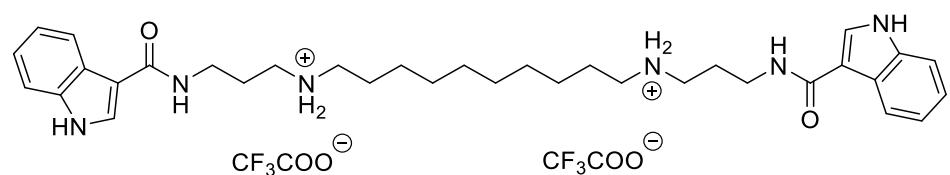
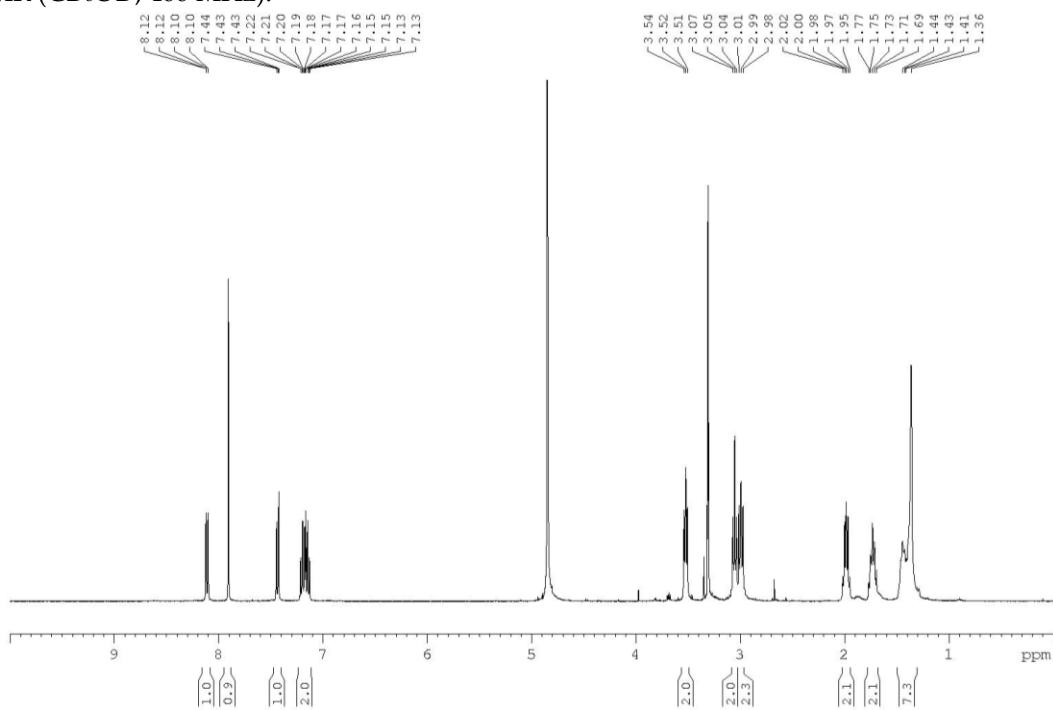


Figure S4 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for 12d



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

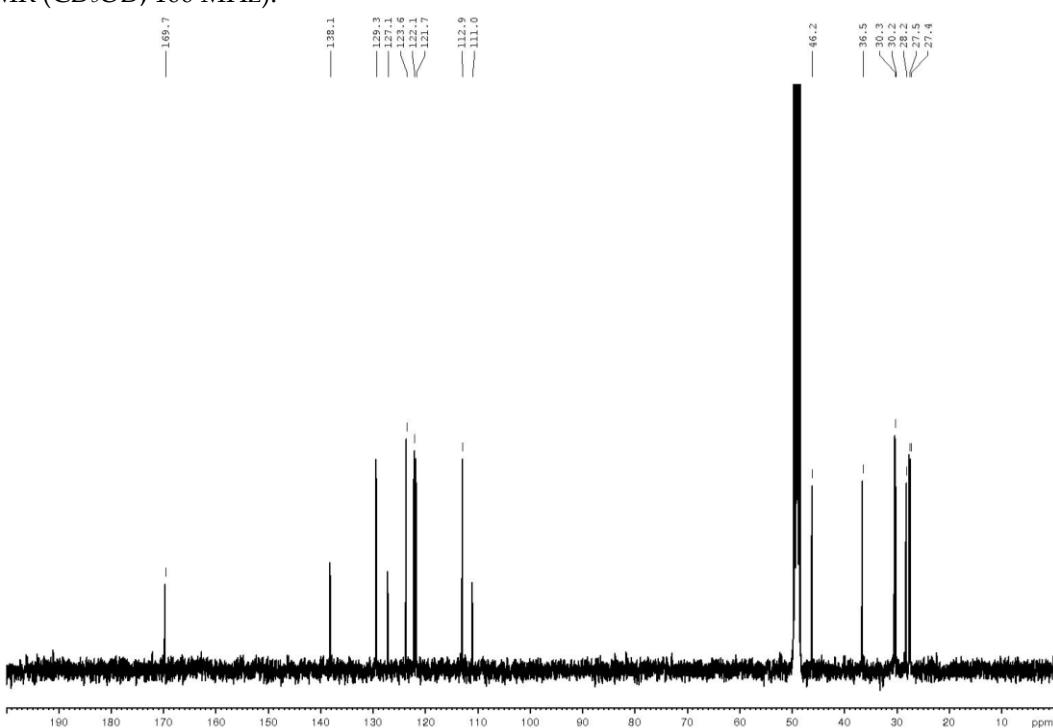
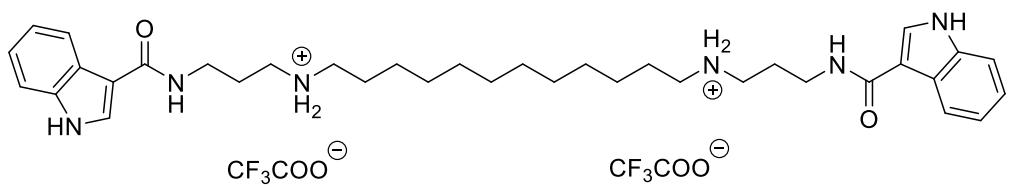
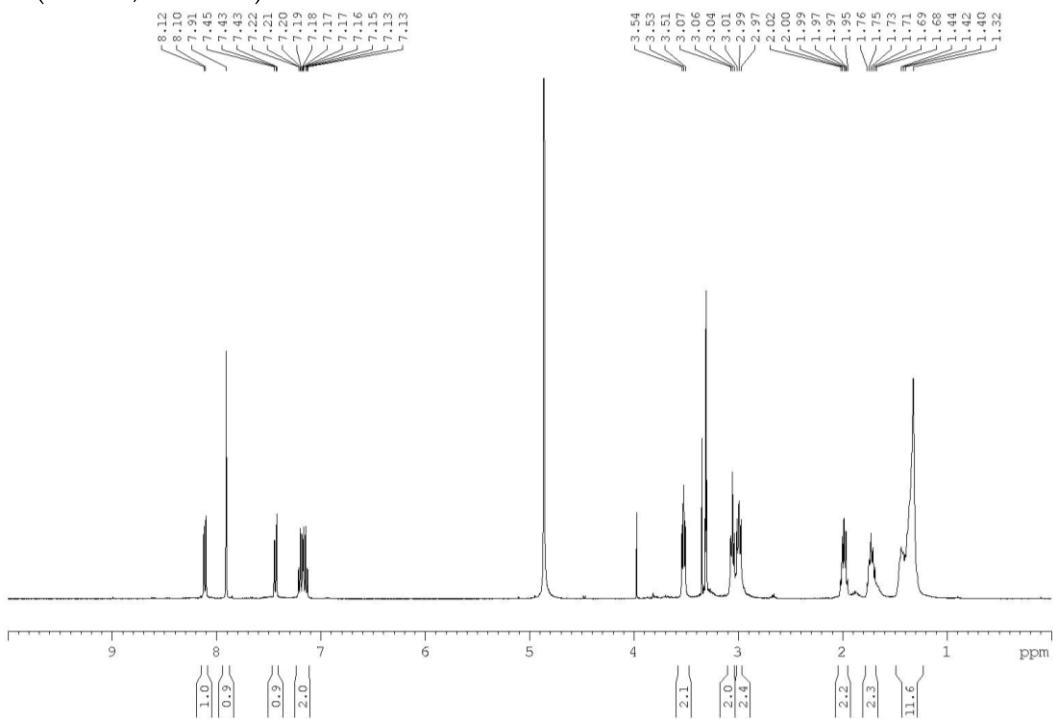


Figure S5 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for 12e



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

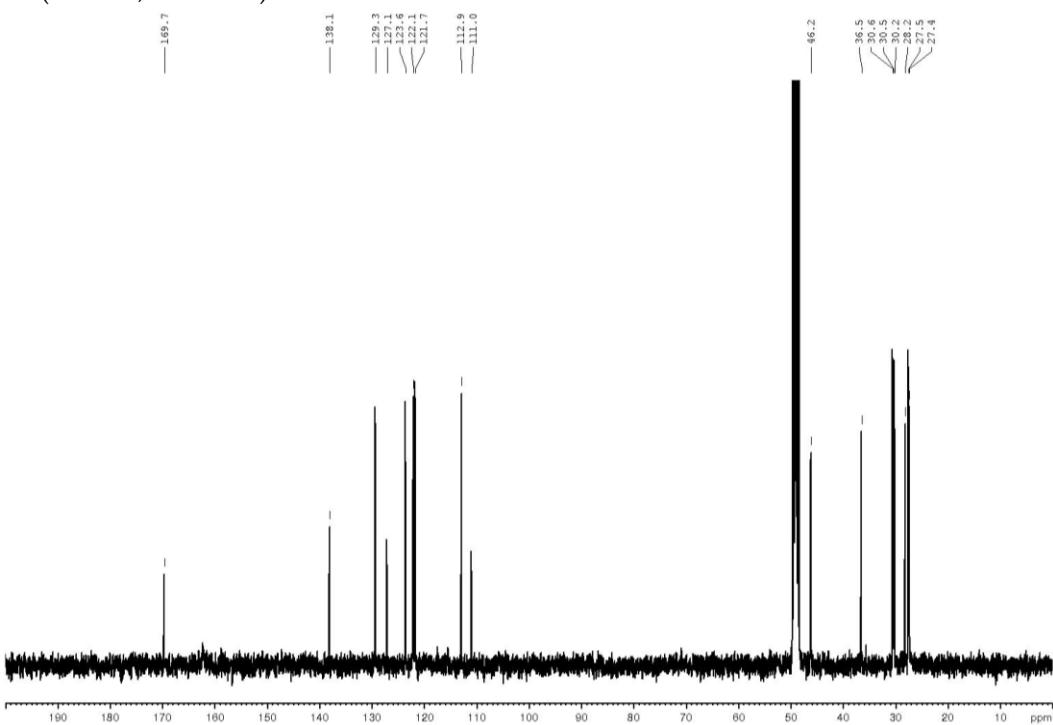
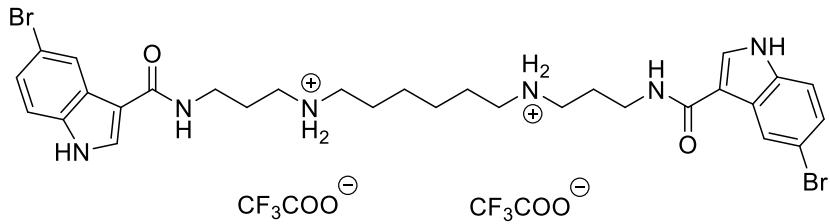
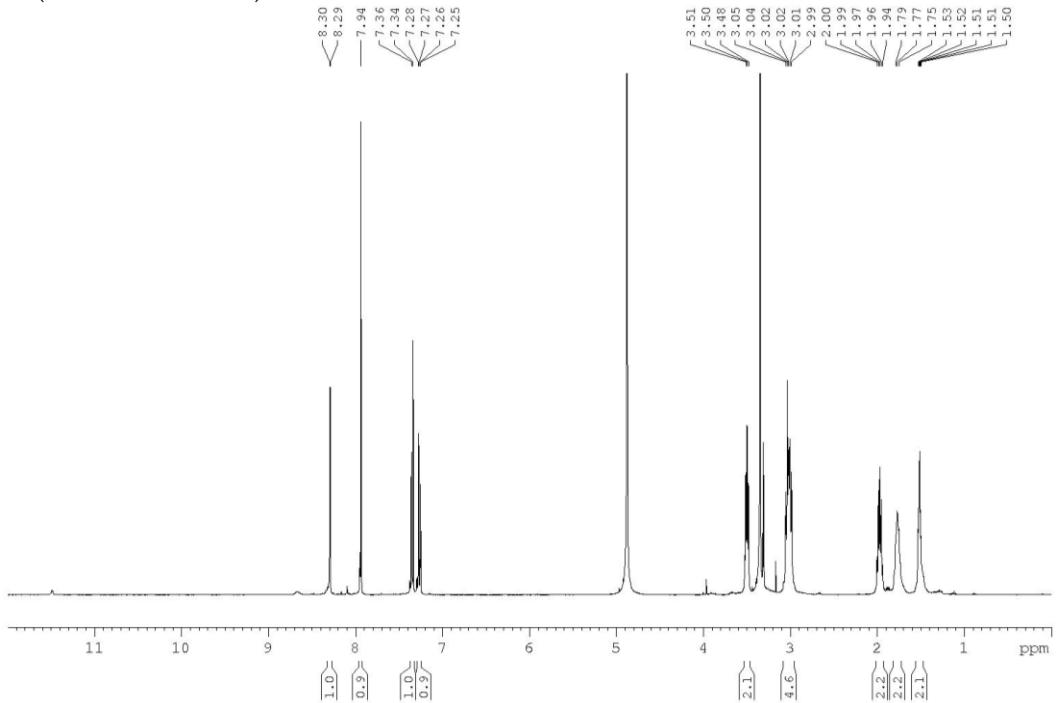


Figure S6 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **12f**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

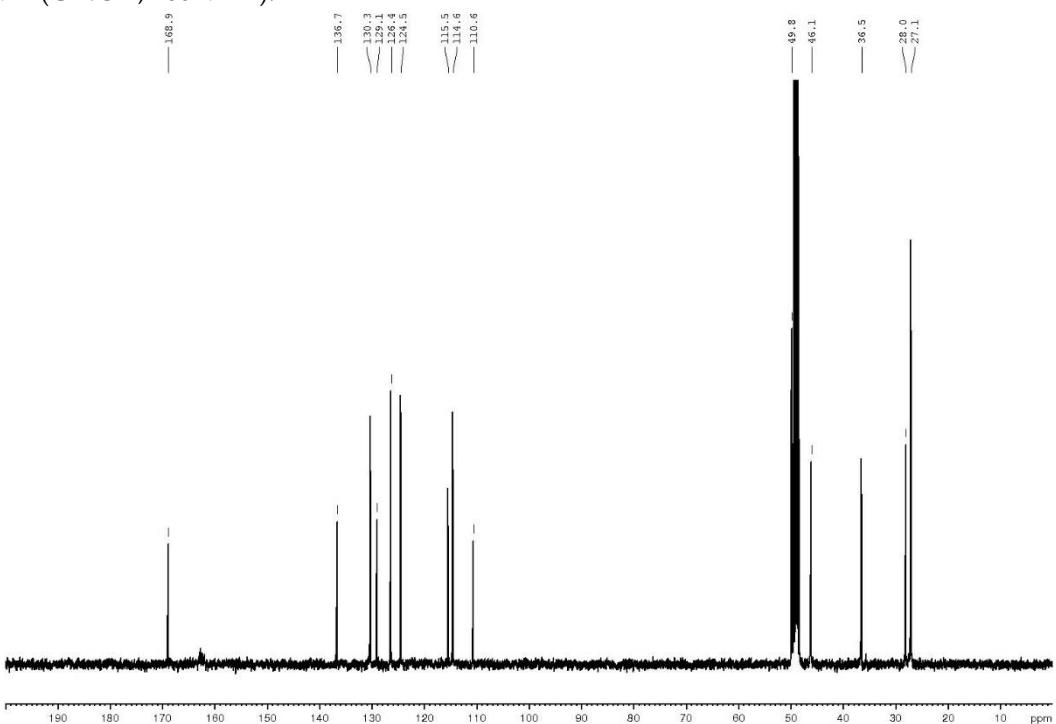
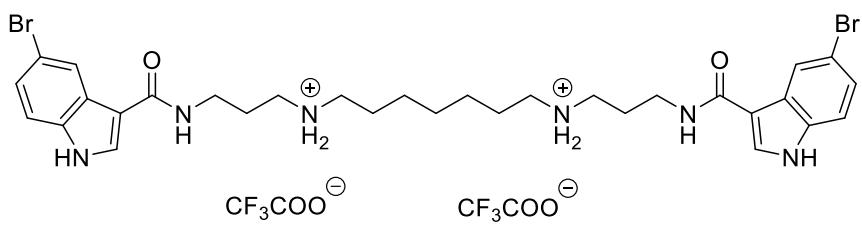
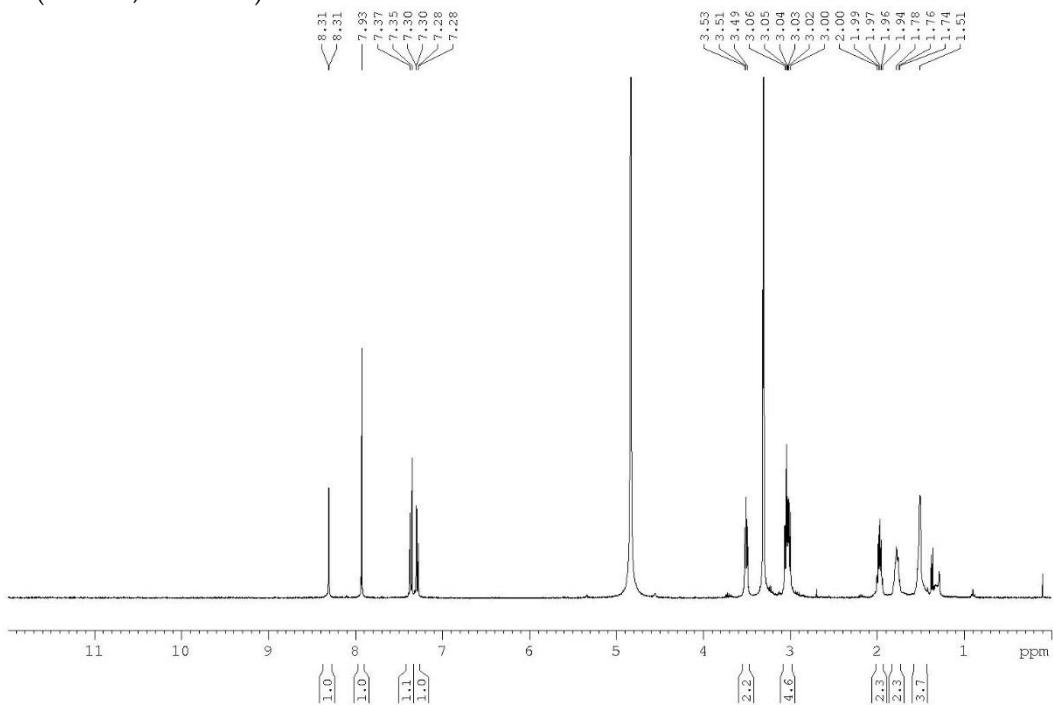


Figure S7 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **13b**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

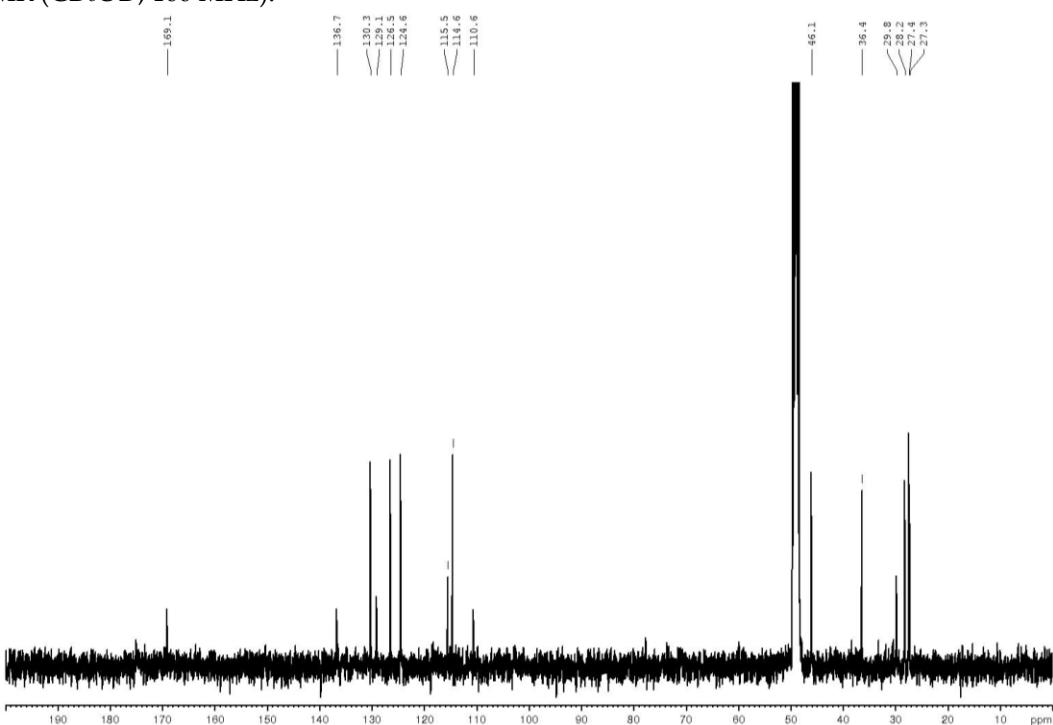
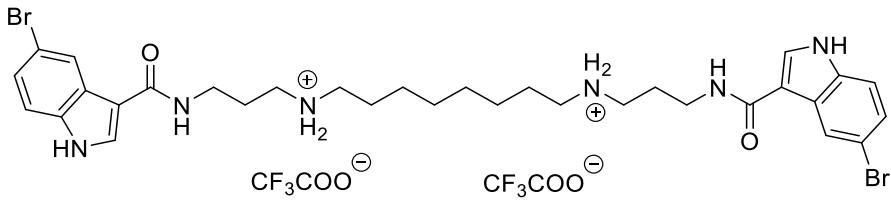
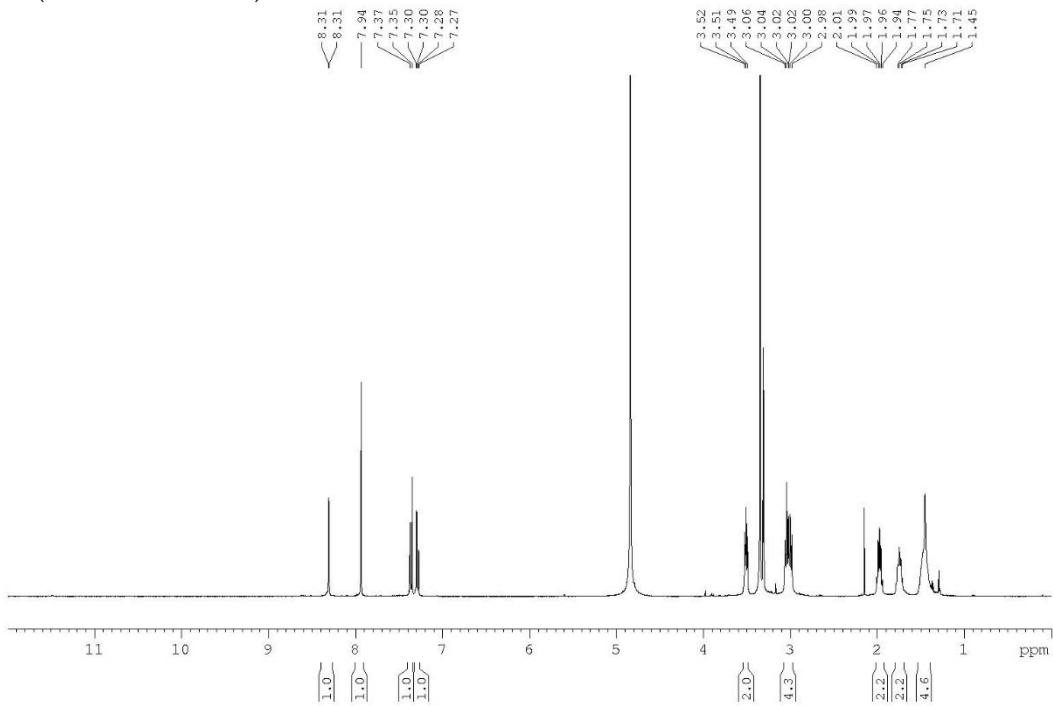


Figure S8 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **13c**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

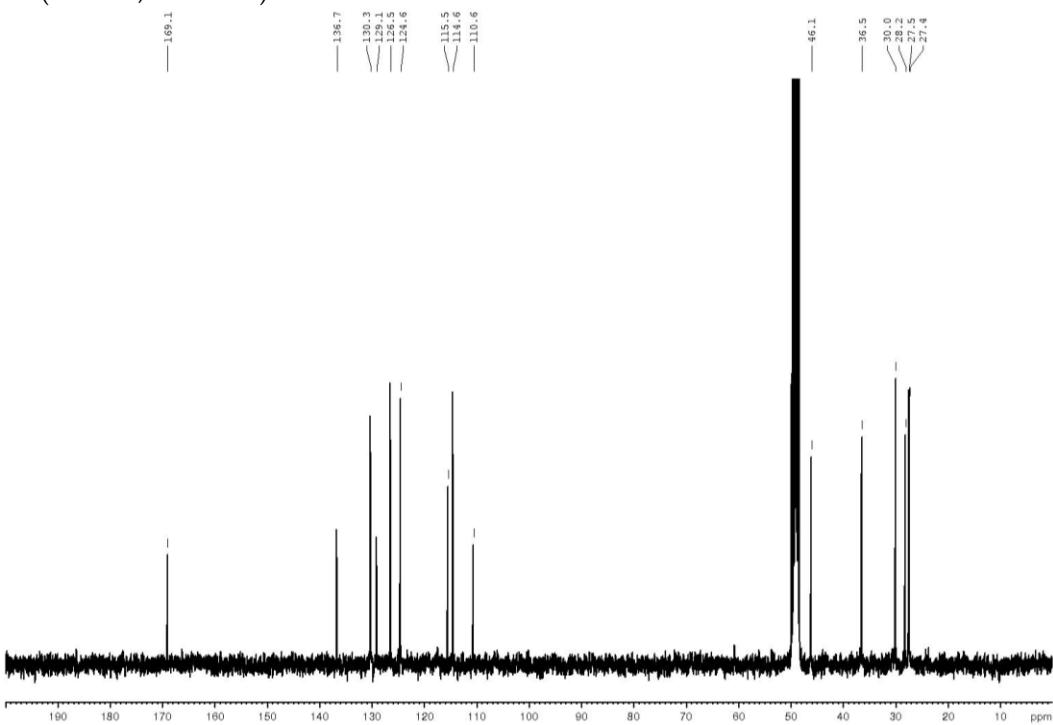
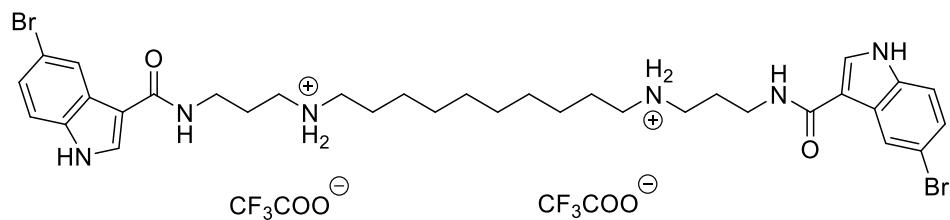
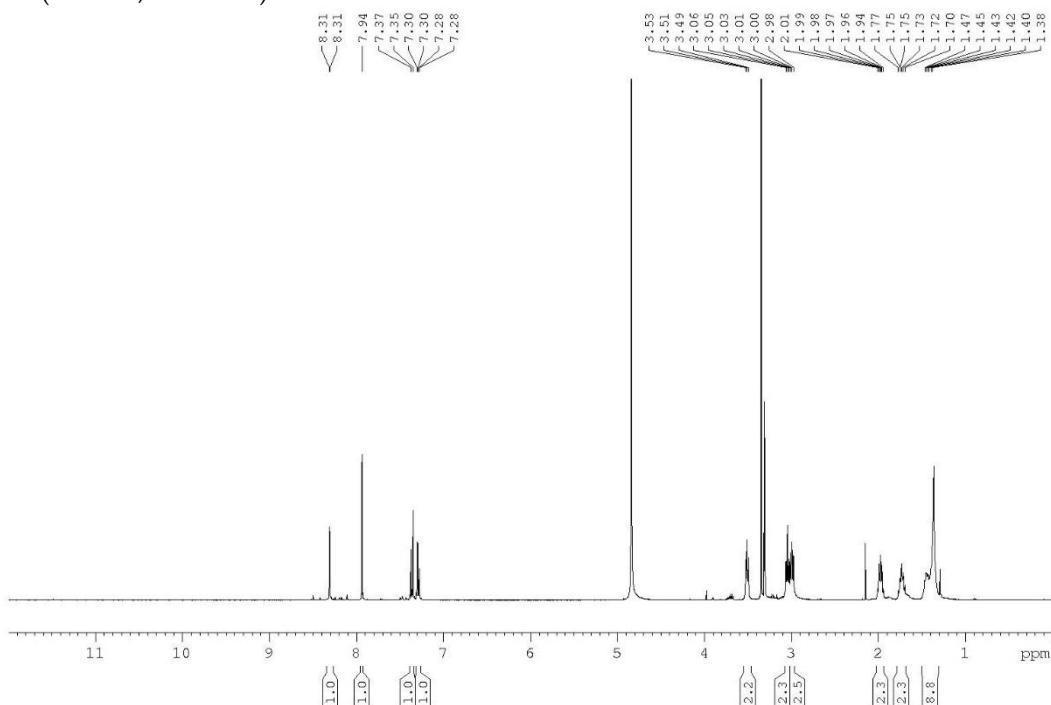


Figure S9 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for 13d



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

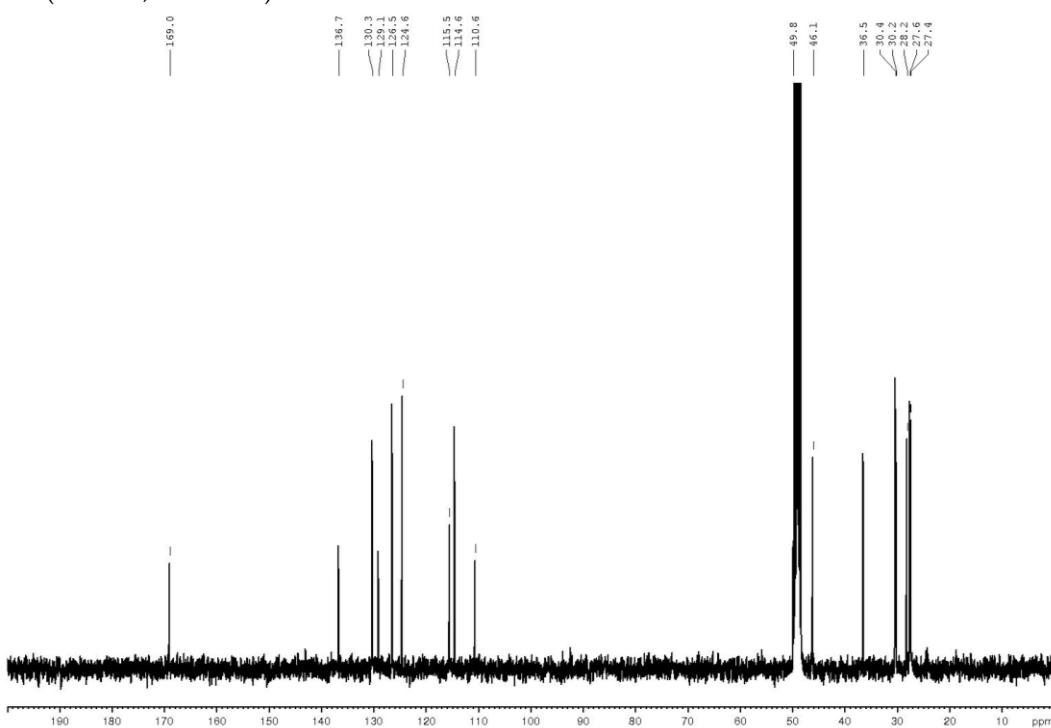
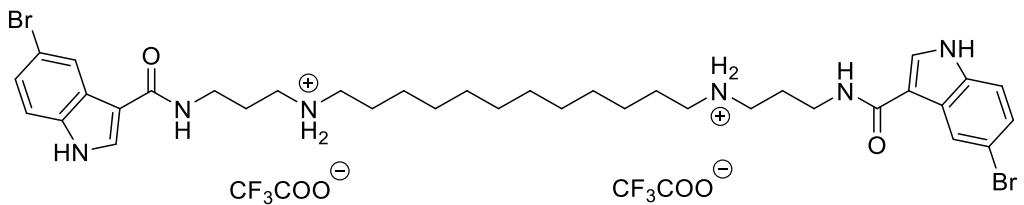
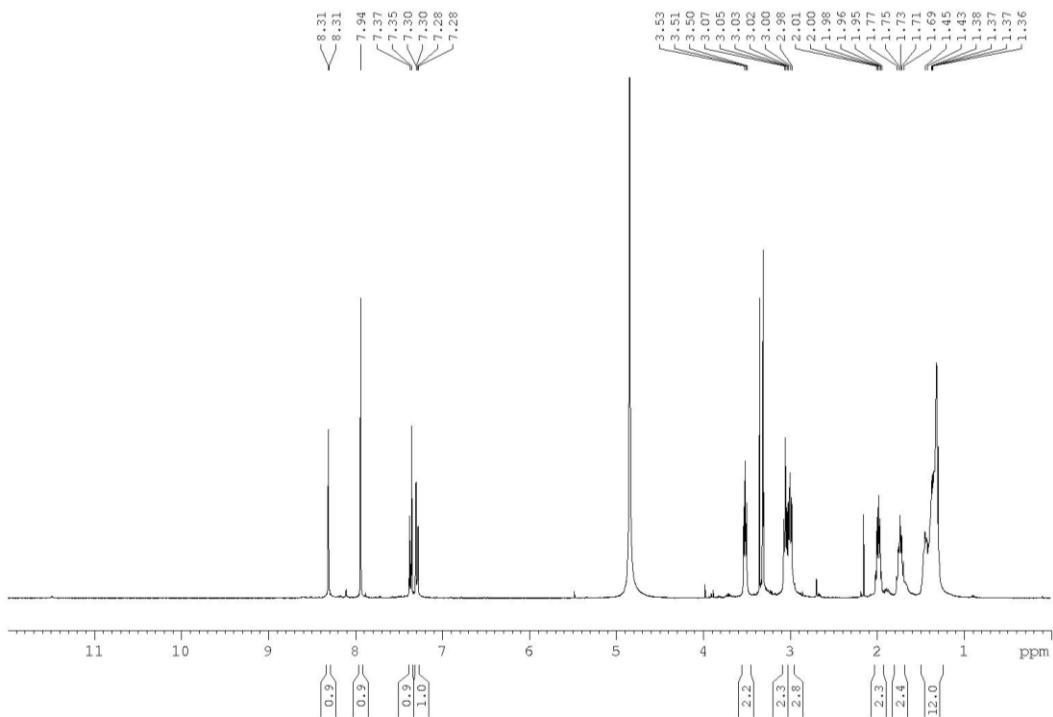


Figure S10 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for 13e



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

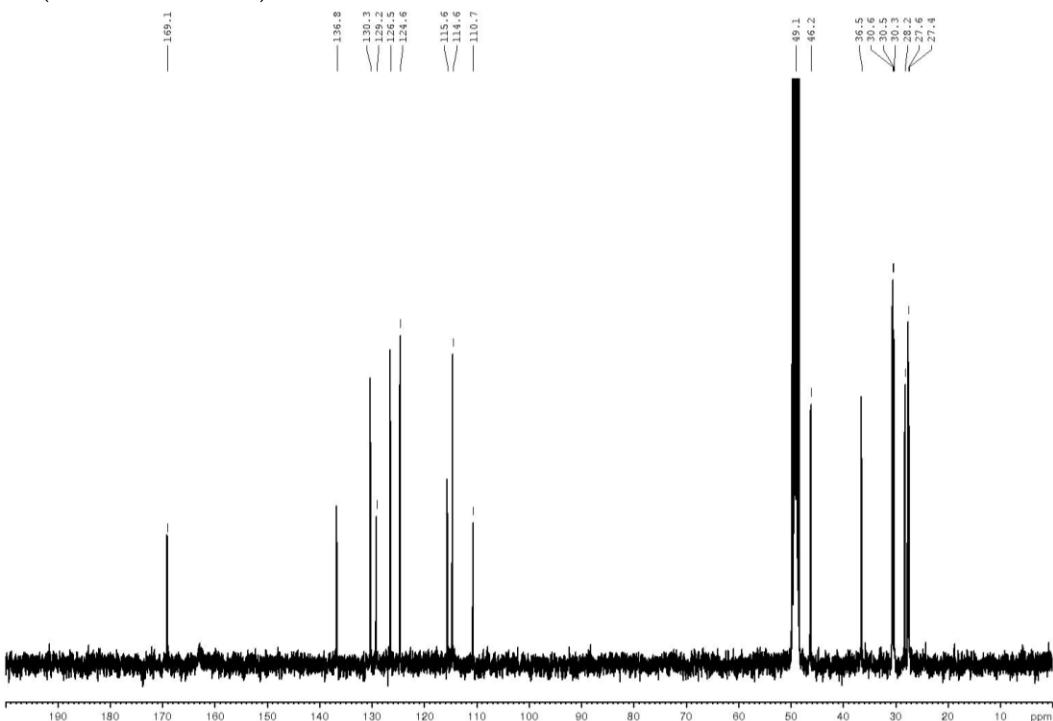
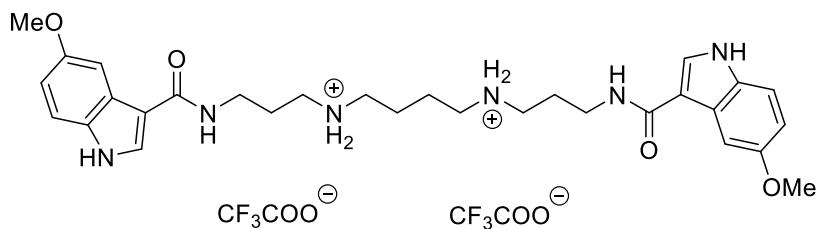


Figure S11 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for 13f



¹H NMR (CD₃OD, 400 MHz):

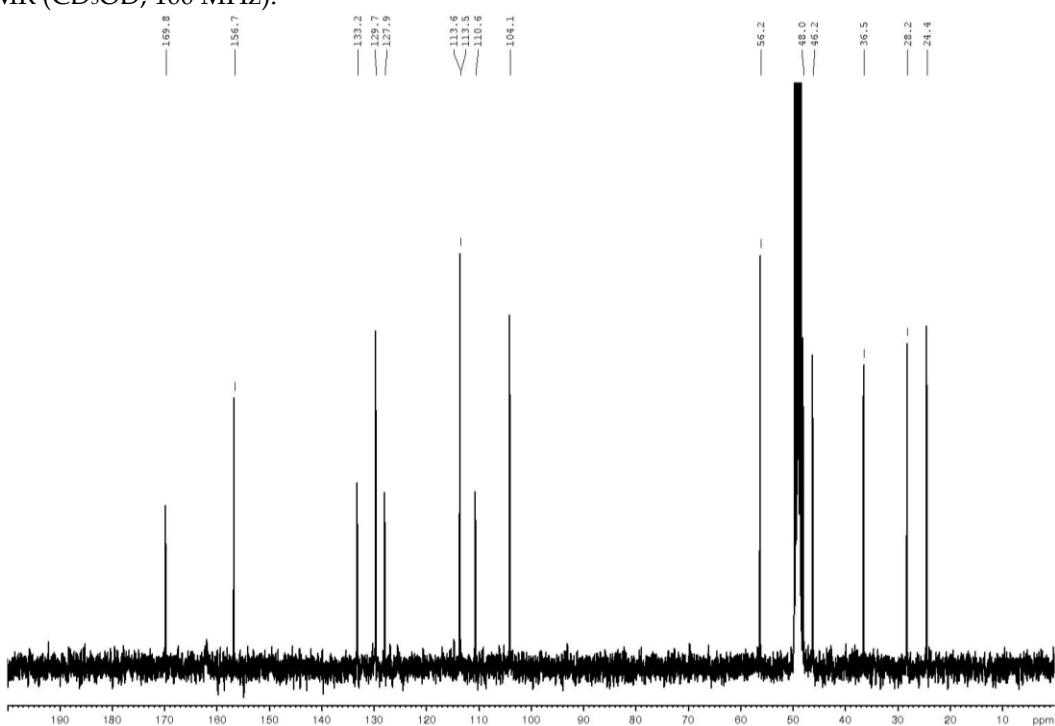
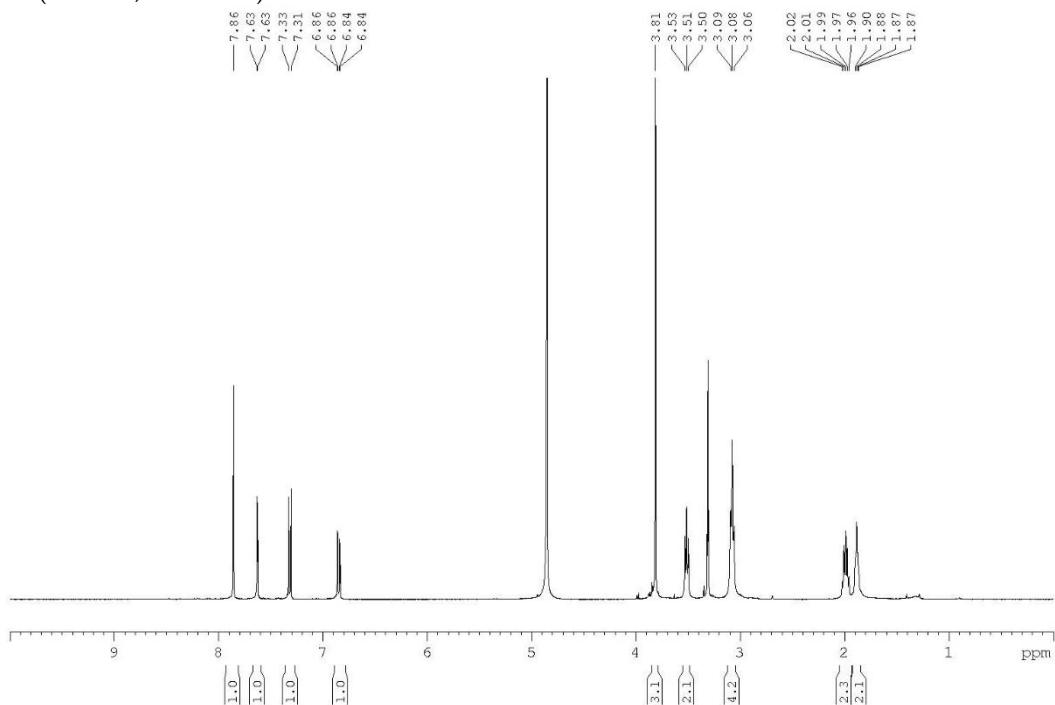
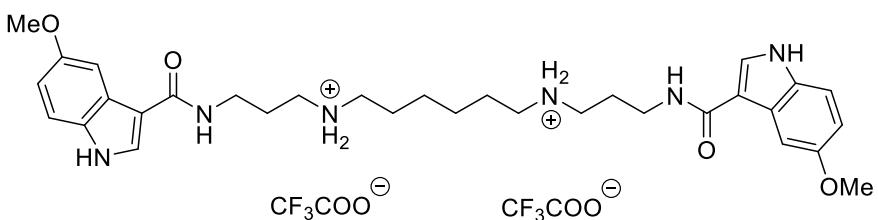
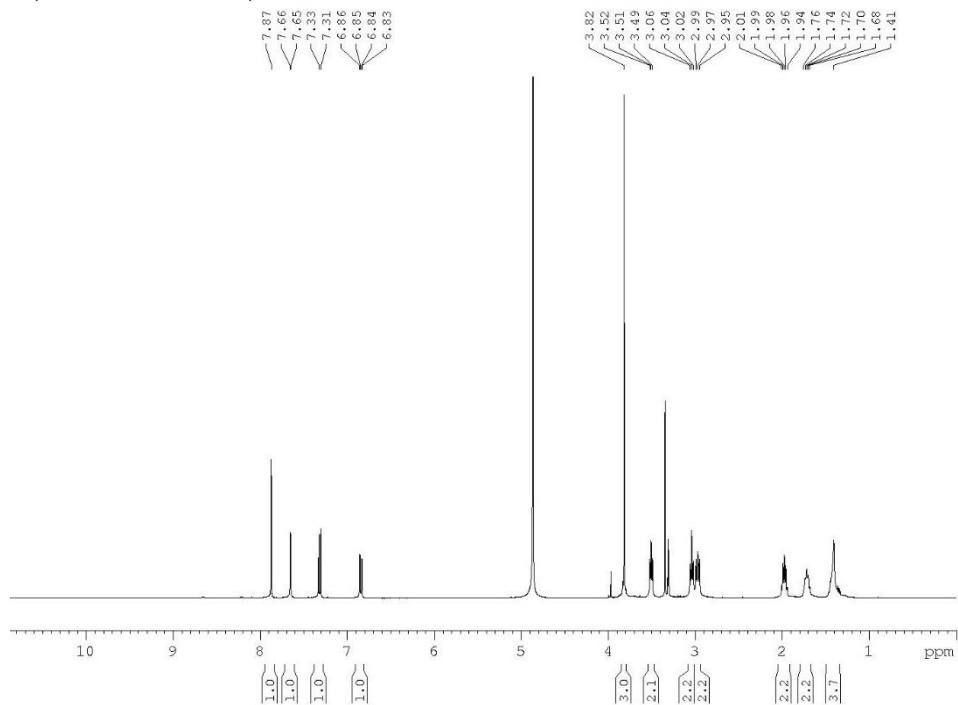


Figure S12 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **14a**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

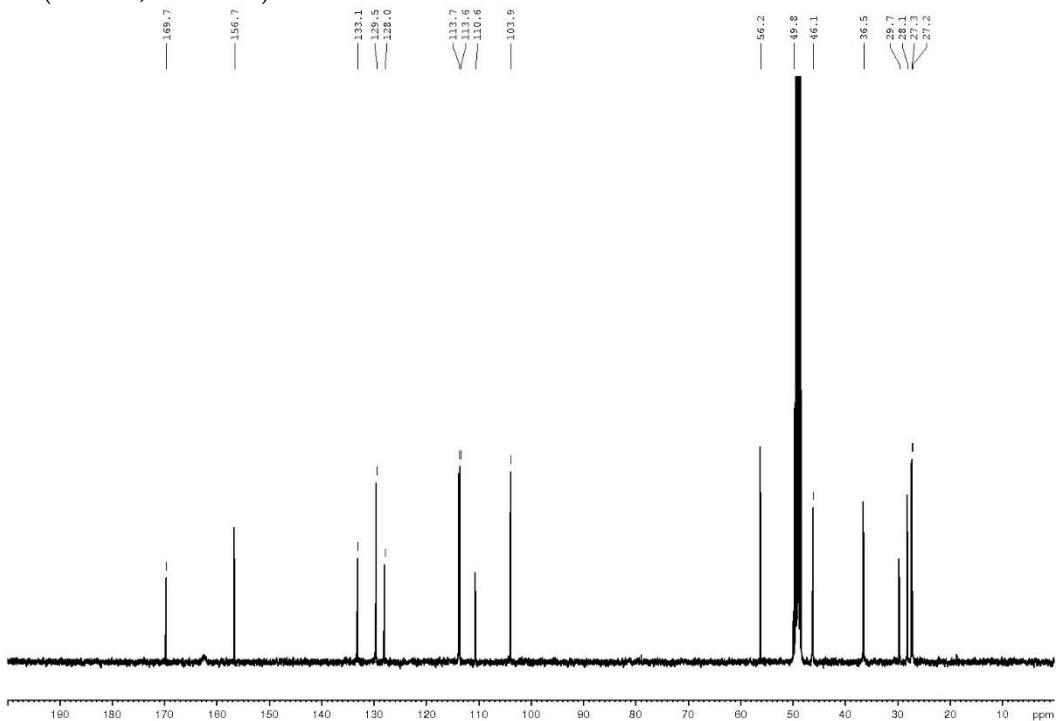
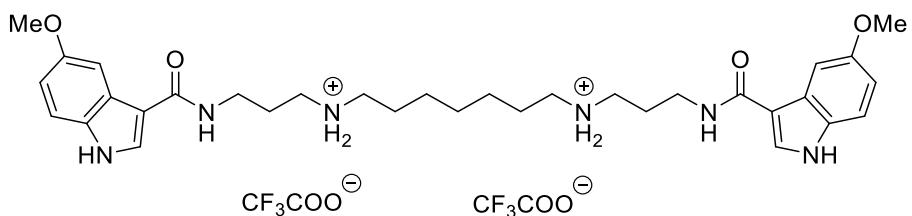
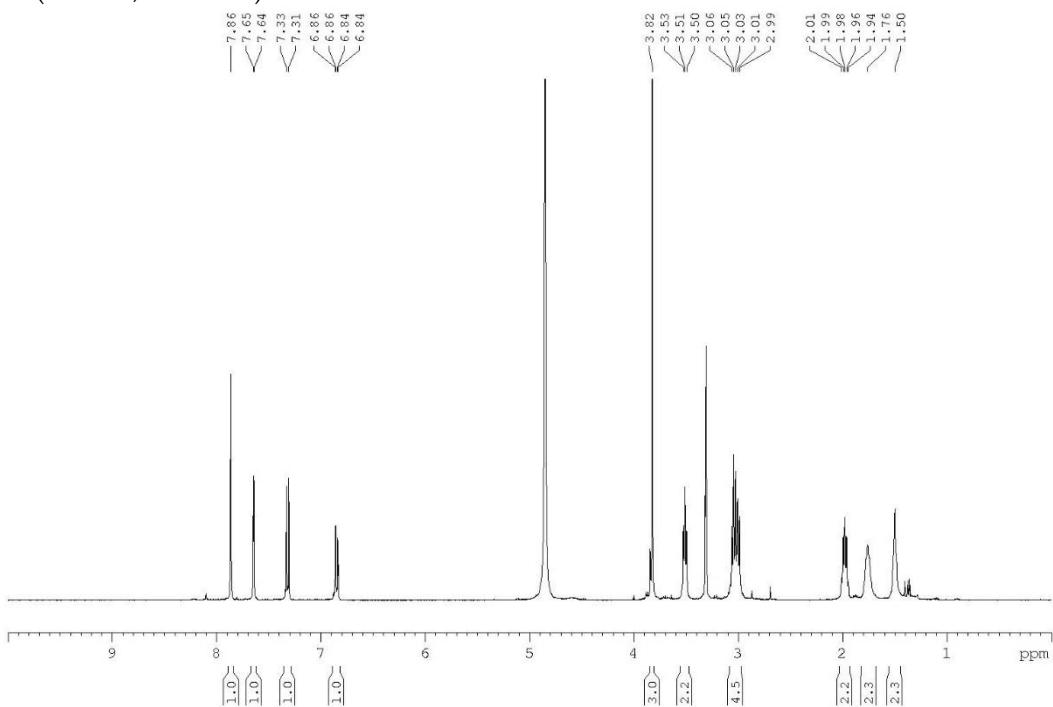


Figure S13 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **14b**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

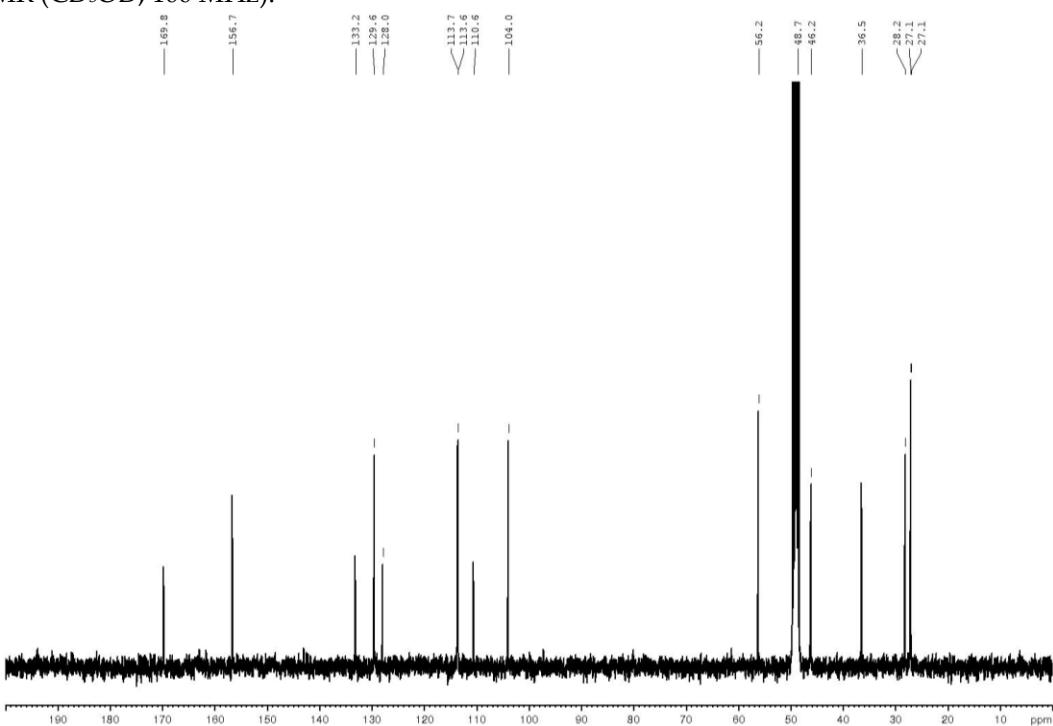
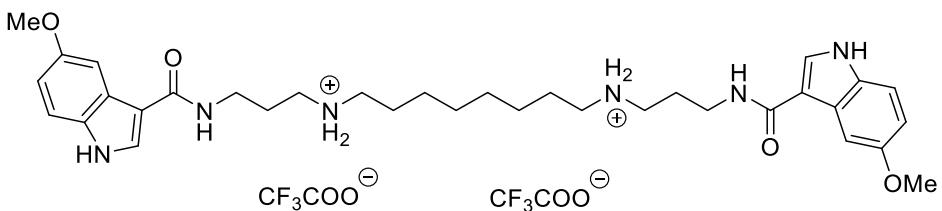
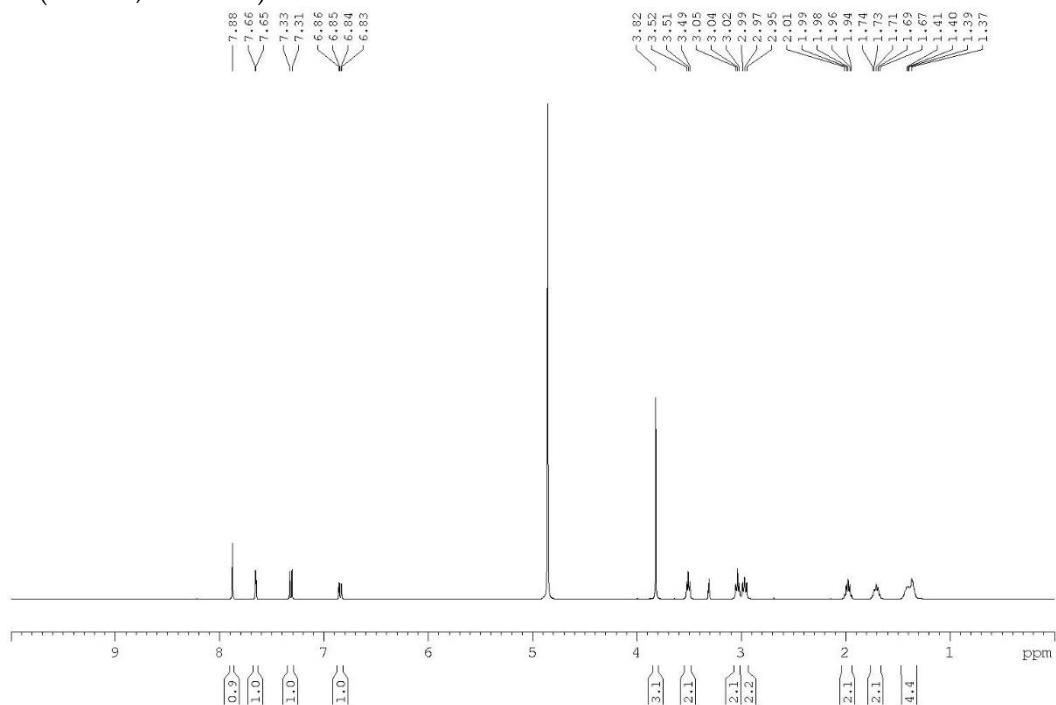


Figure S14 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **14c**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

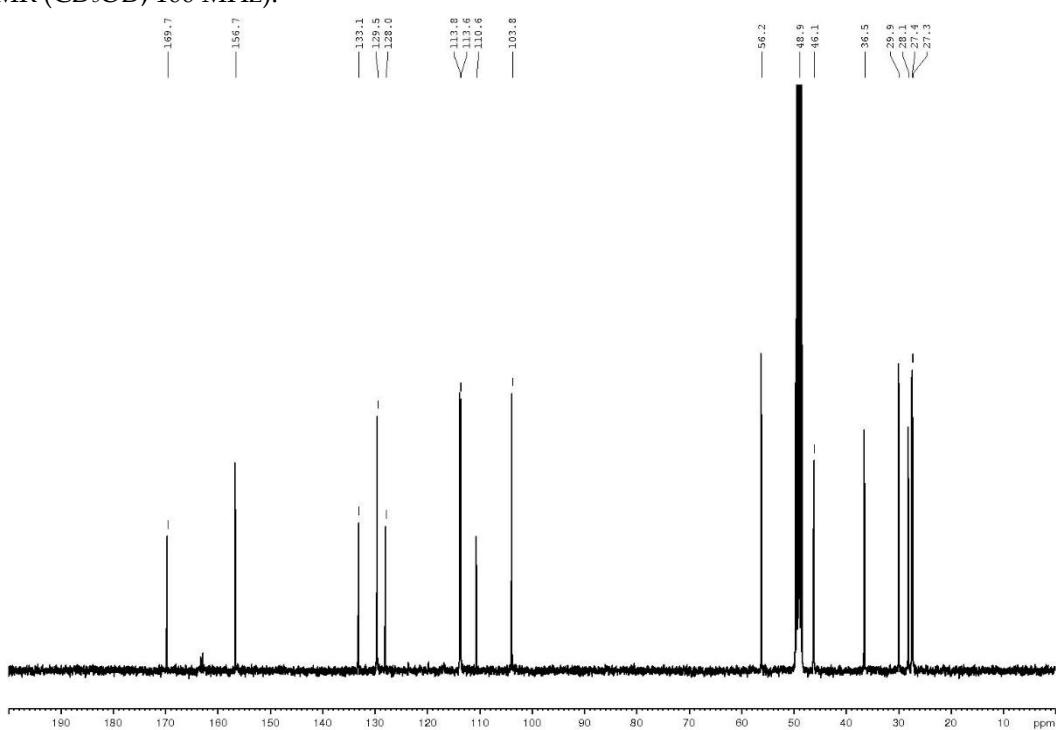
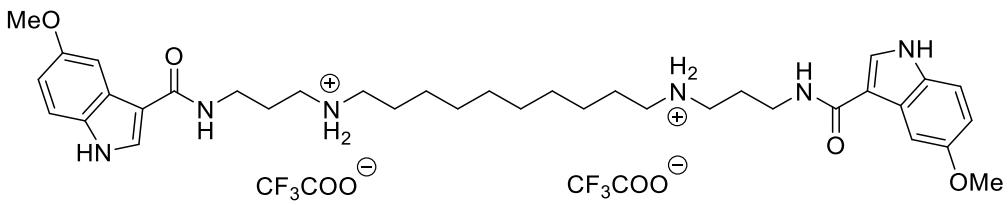
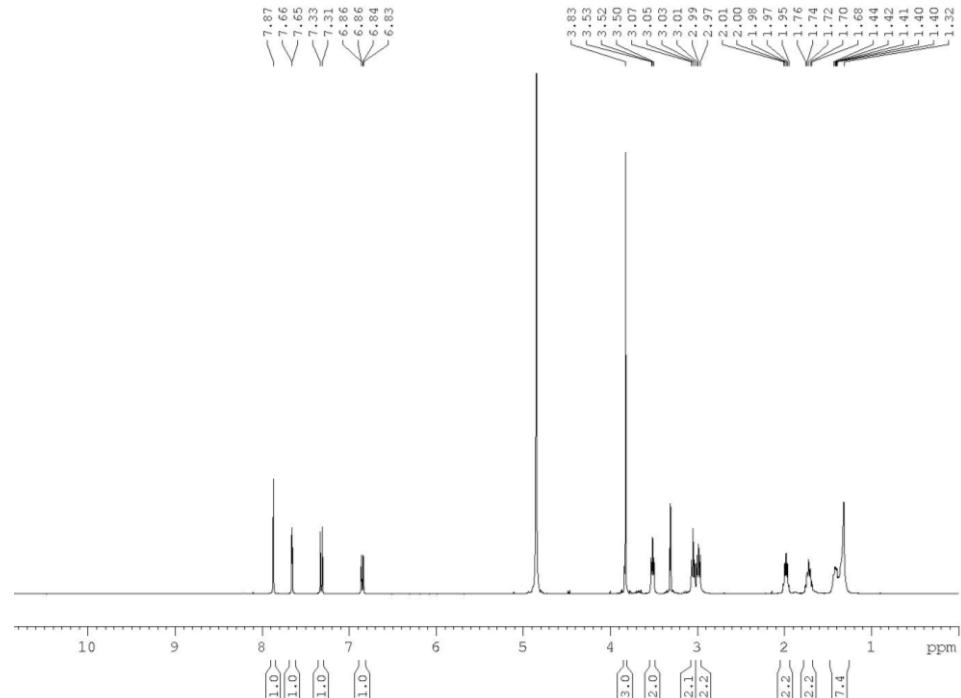


Figure S15 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **14d**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

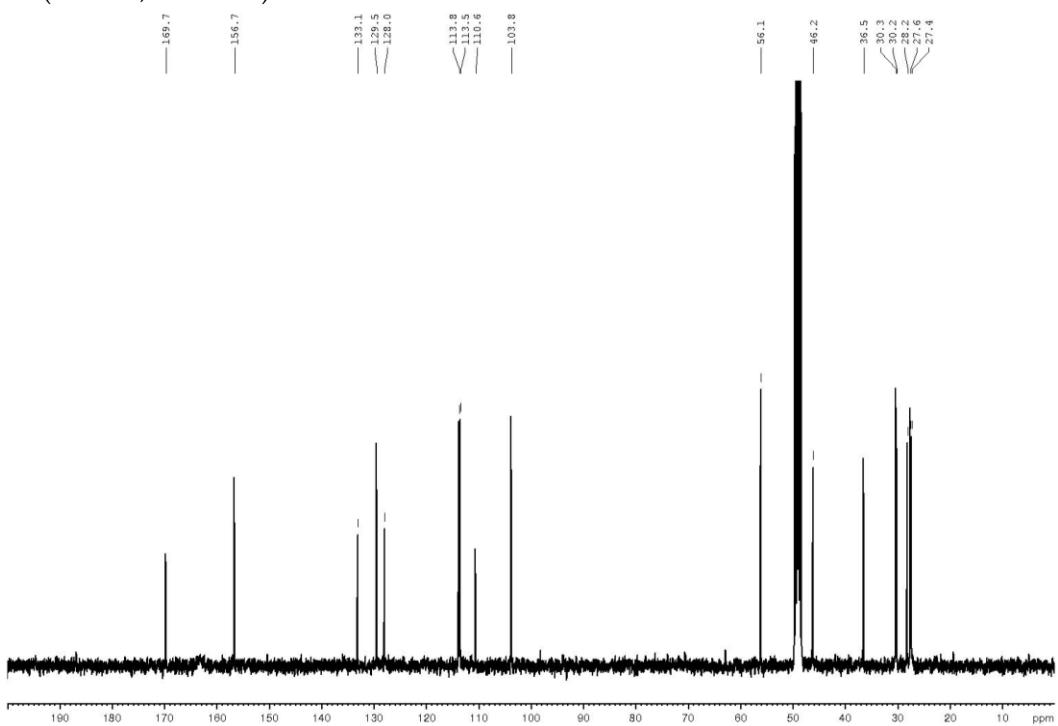
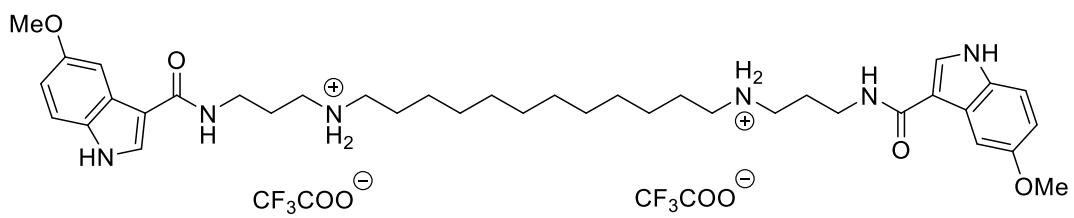
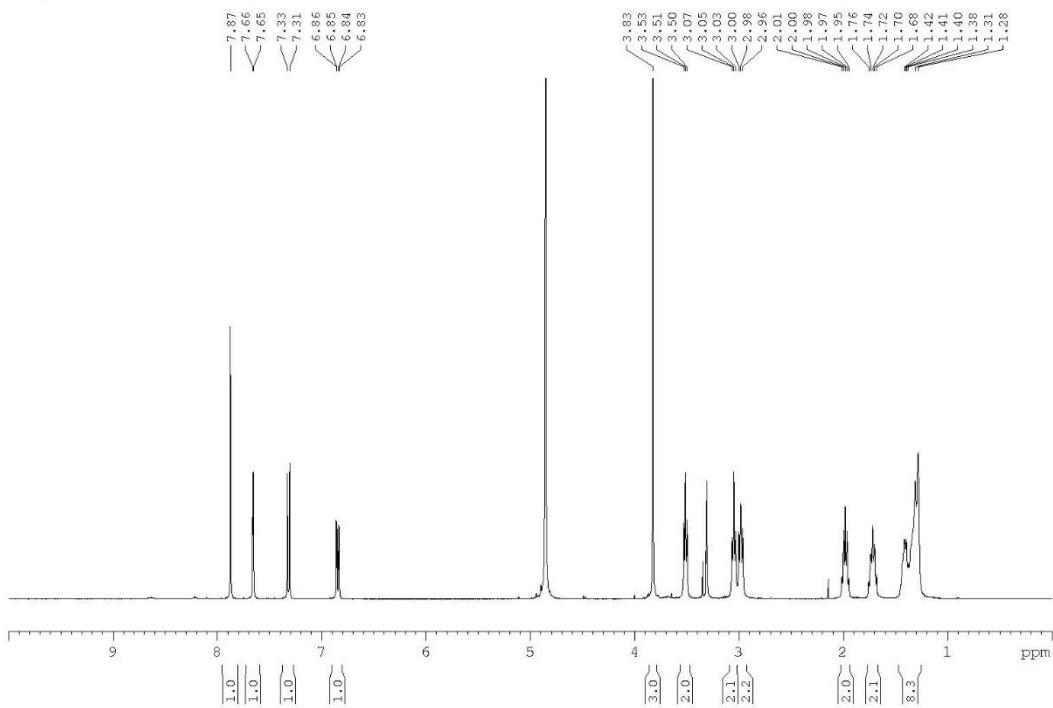


Figure S16 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **14e**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

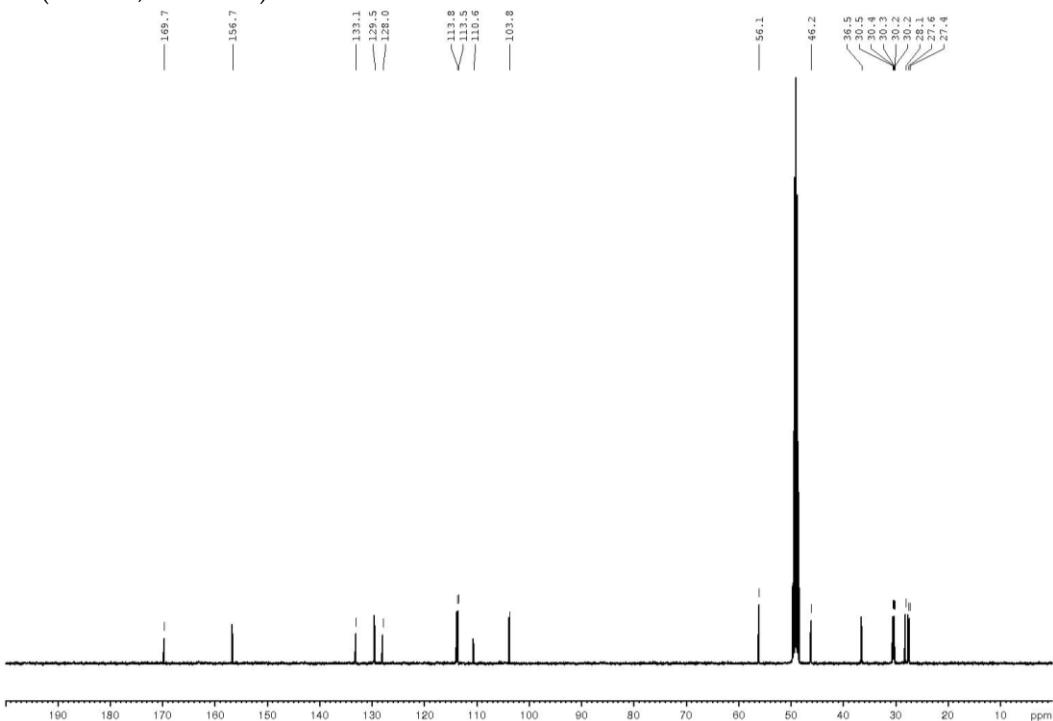
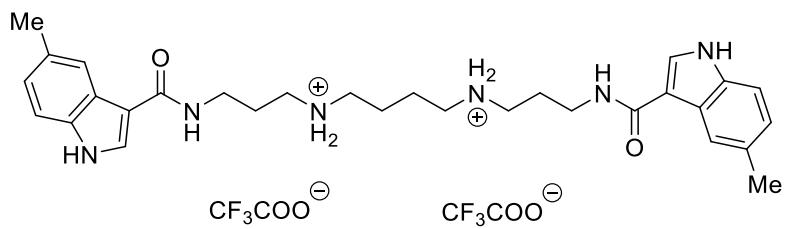
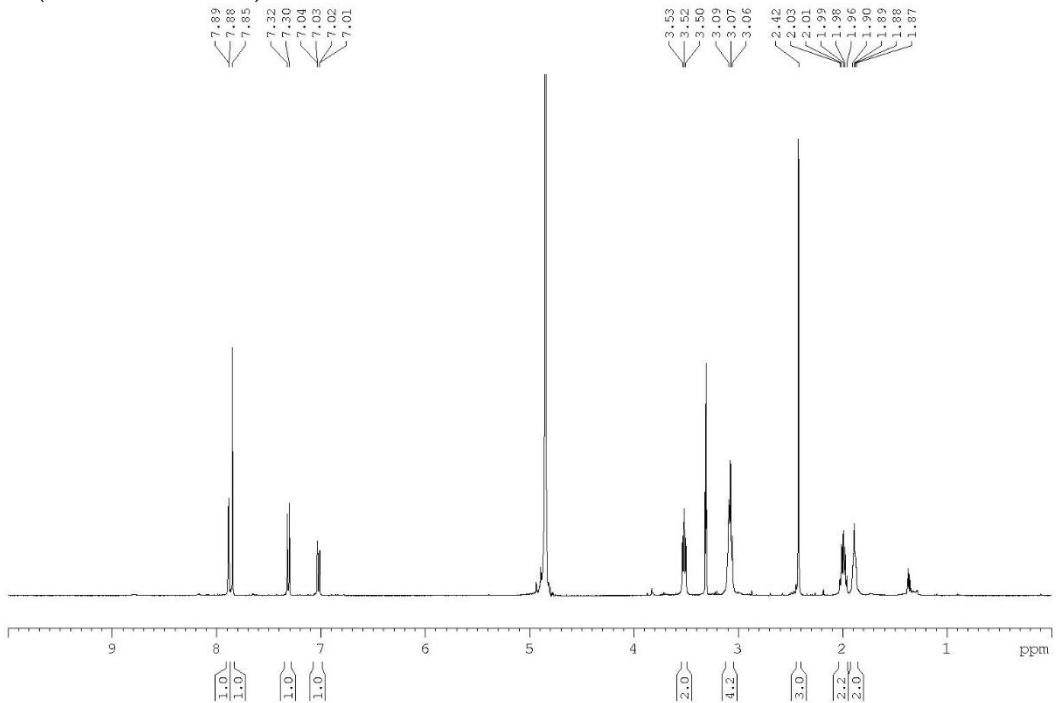


Figure S17 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **14f**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

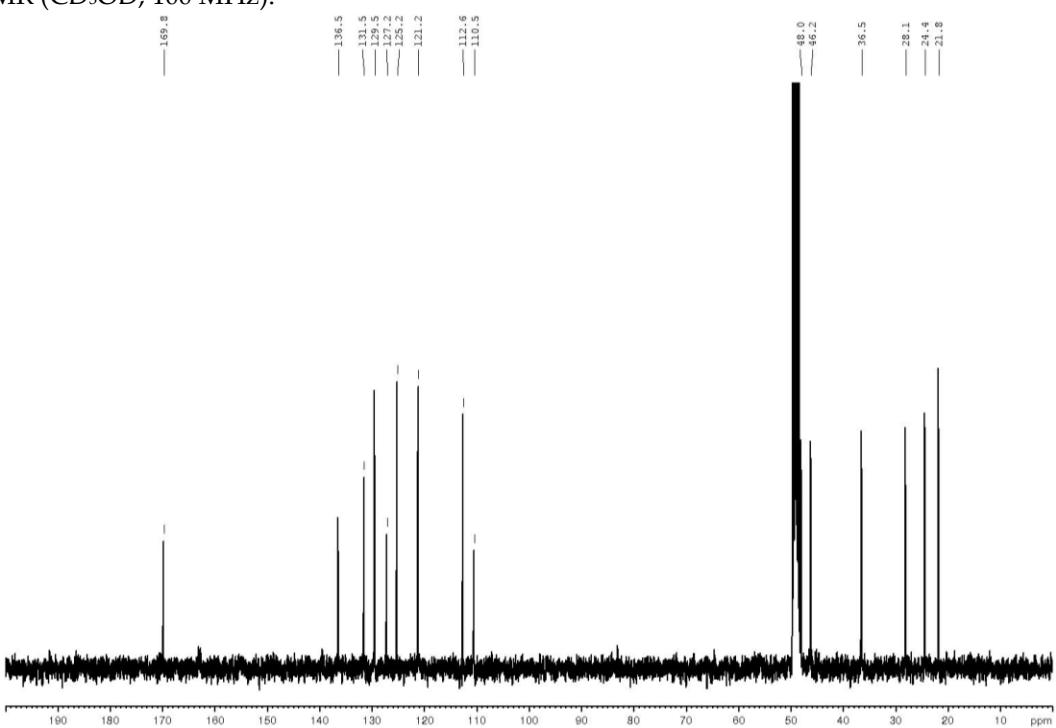
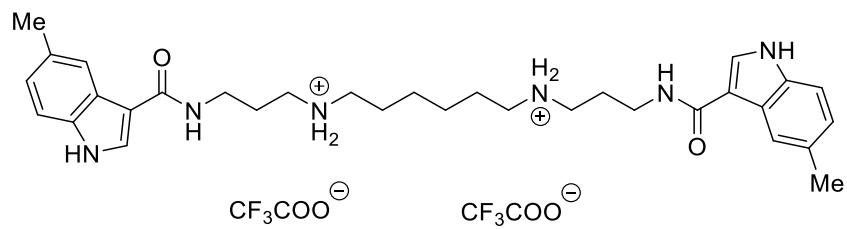
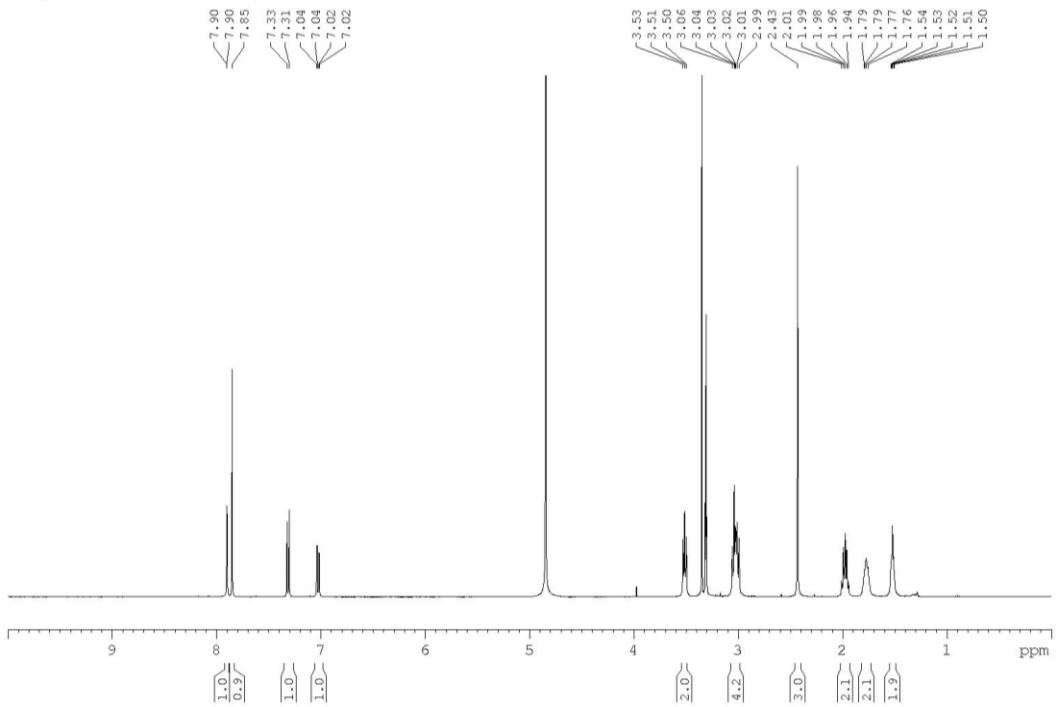


Figure S18 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **15a**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

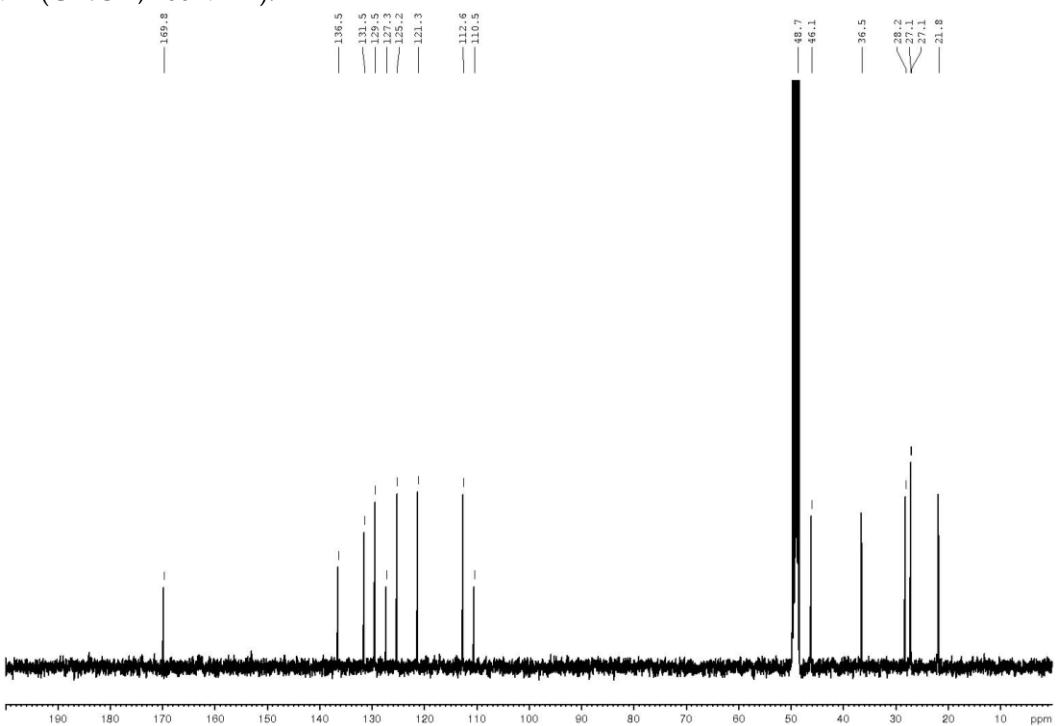
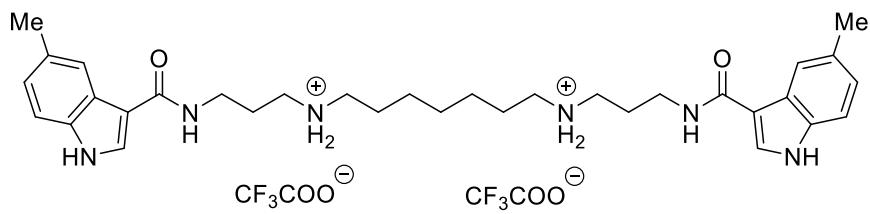
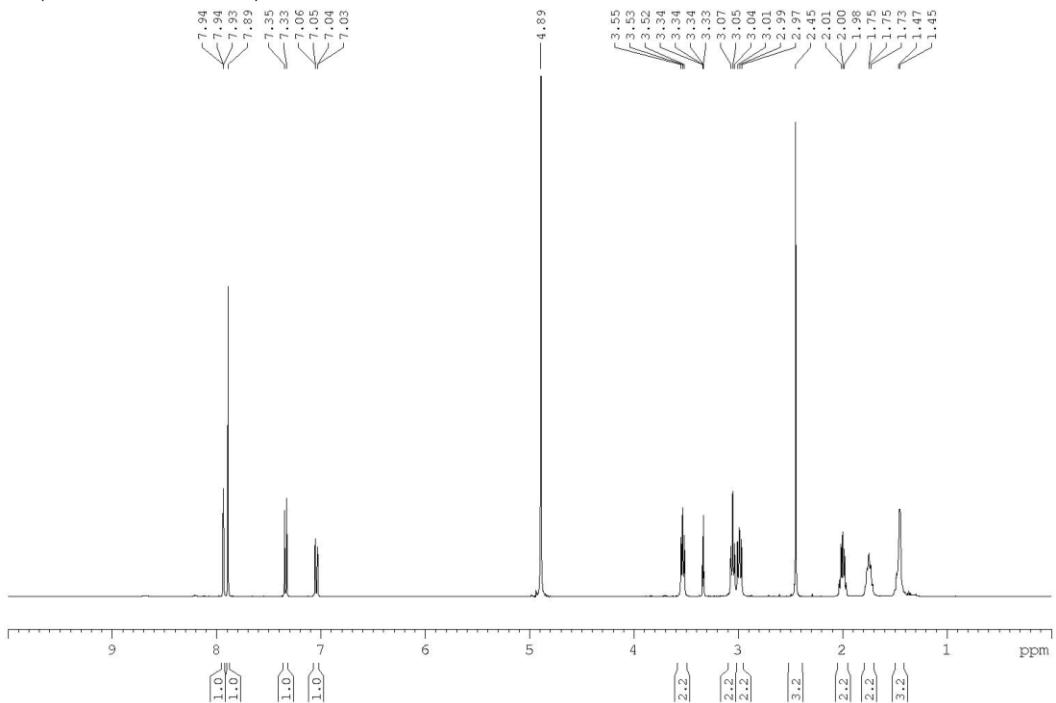


Figure S19 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **15b**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

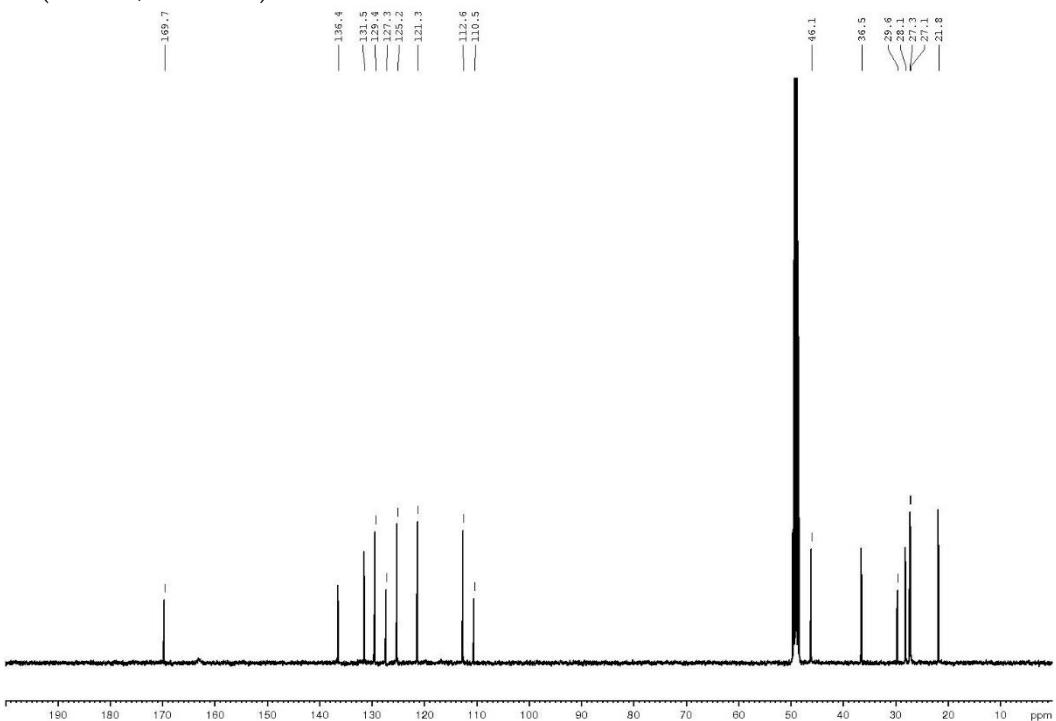
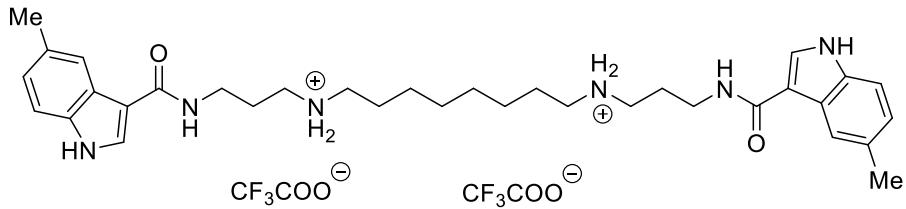
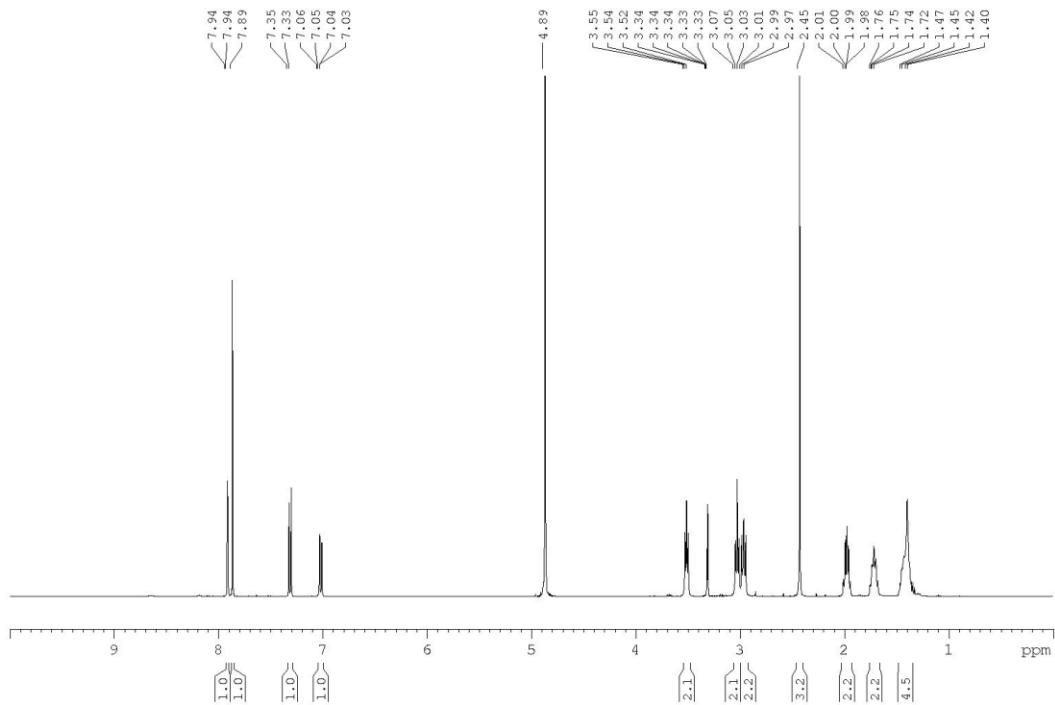


Figure S20 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **15c**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

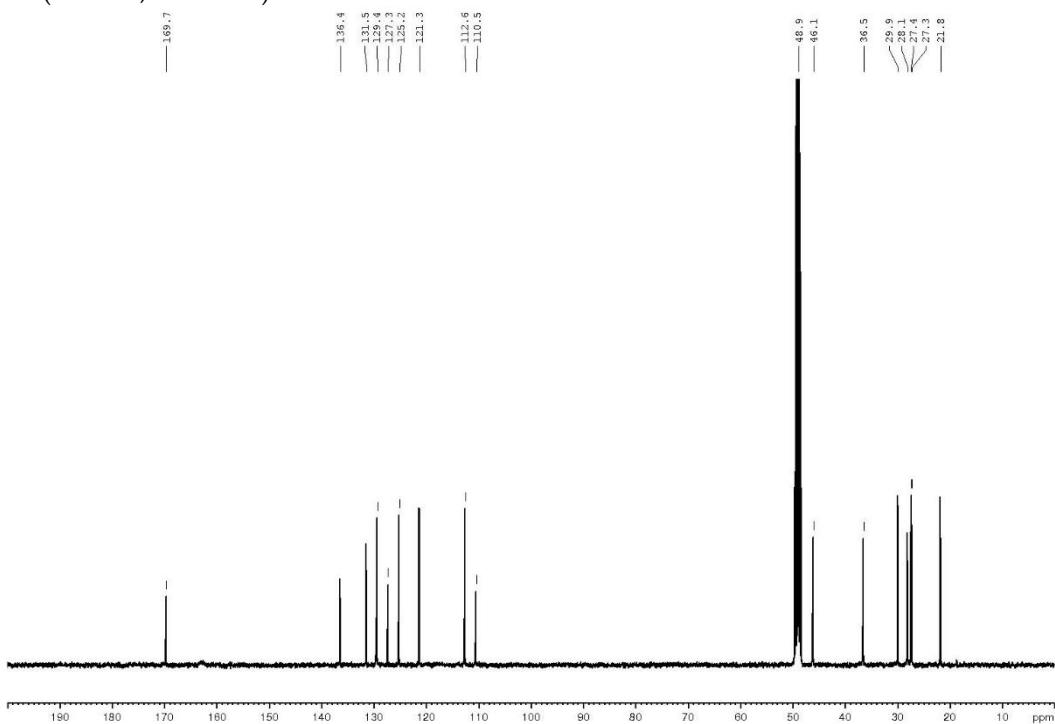
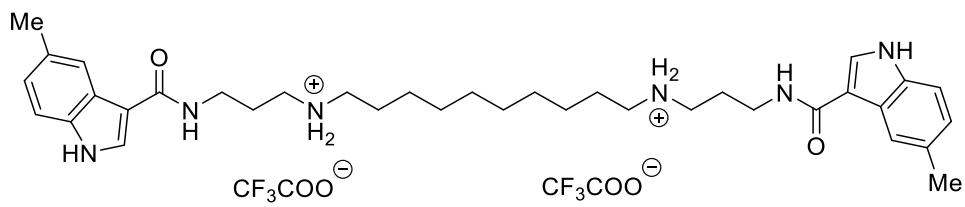
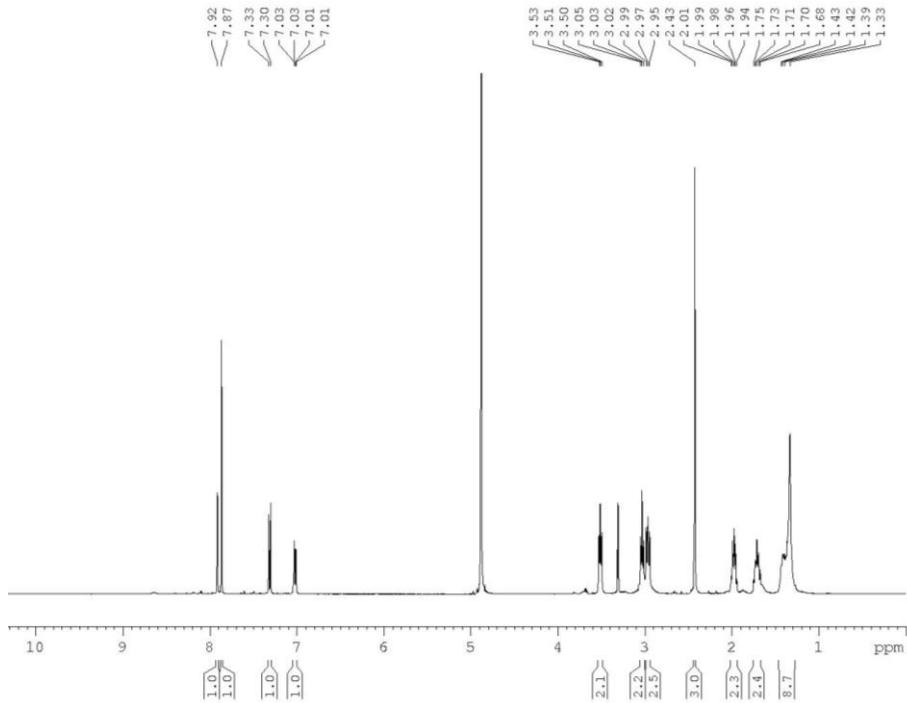


Figure S21 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **15d**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

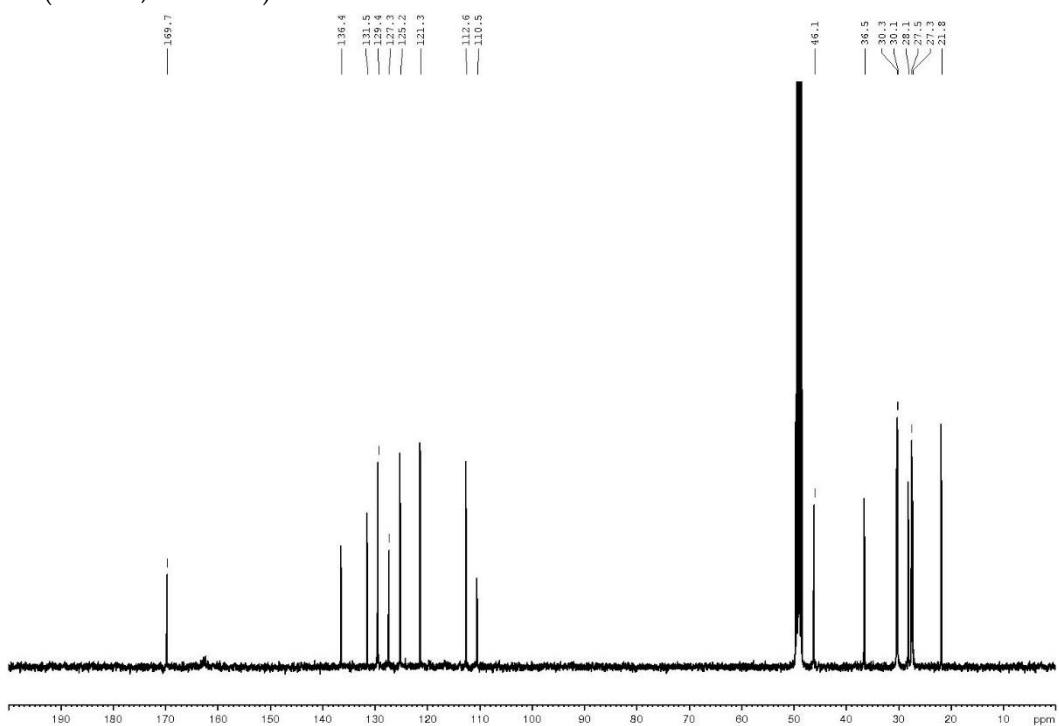
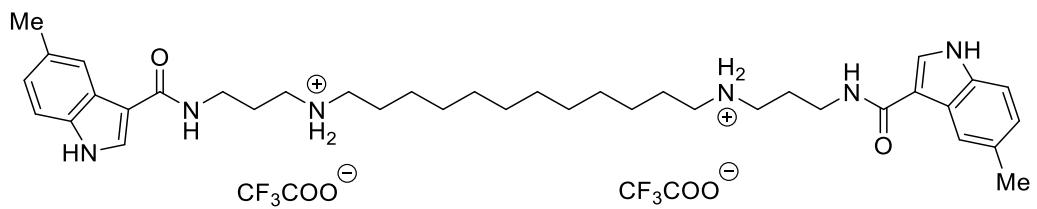
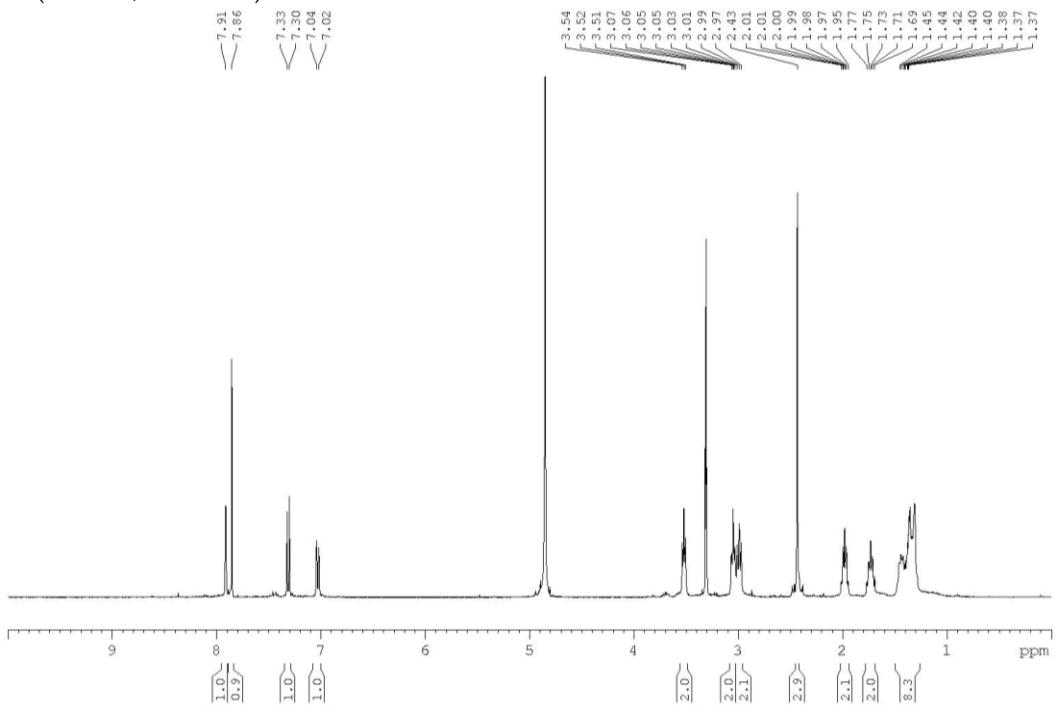


Figure S22 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **15e**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

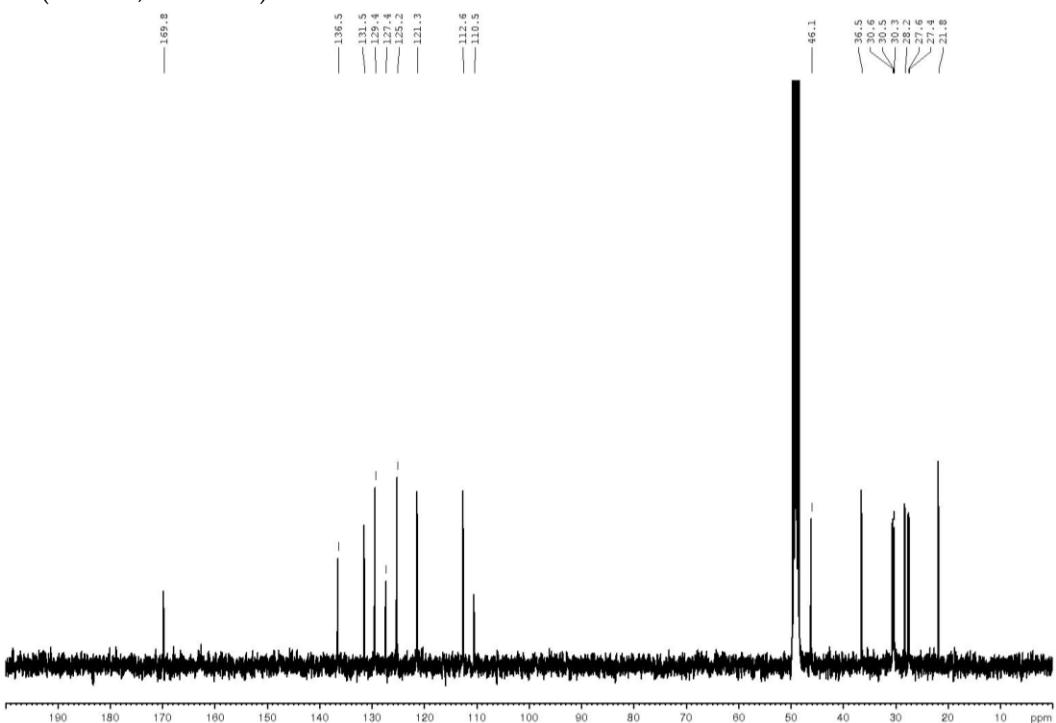
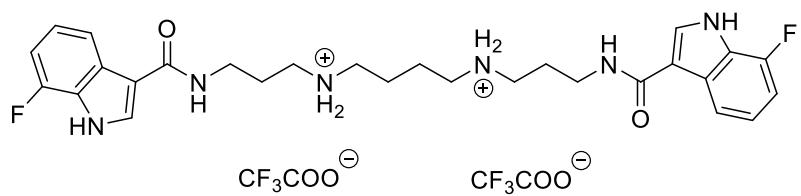
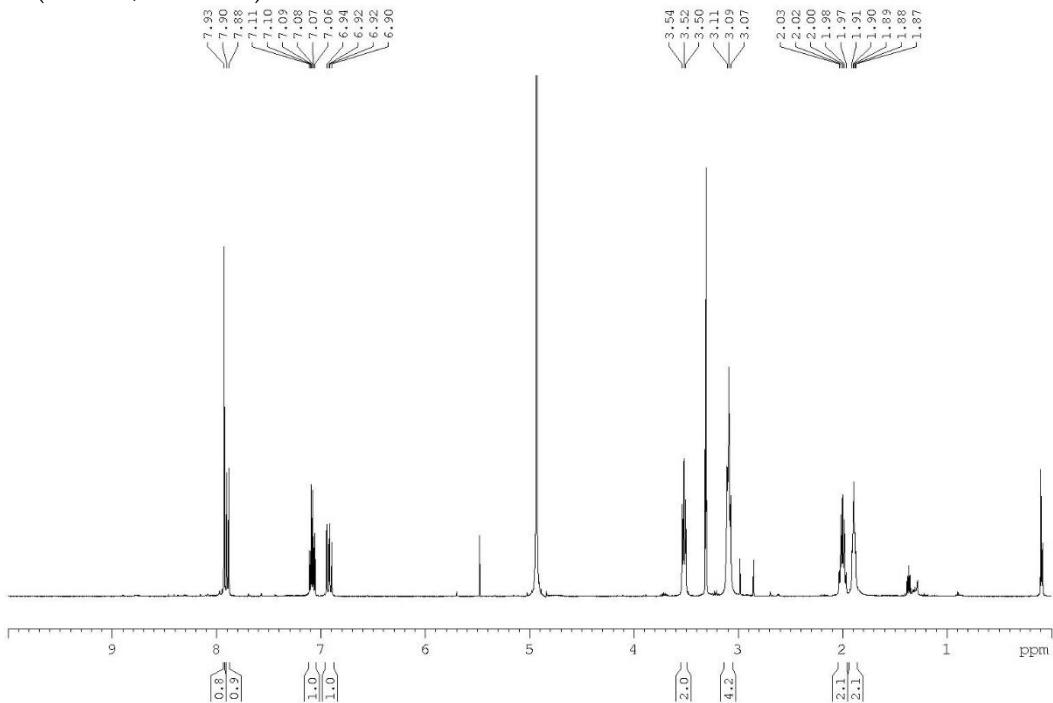


Figure S23 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **15f**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

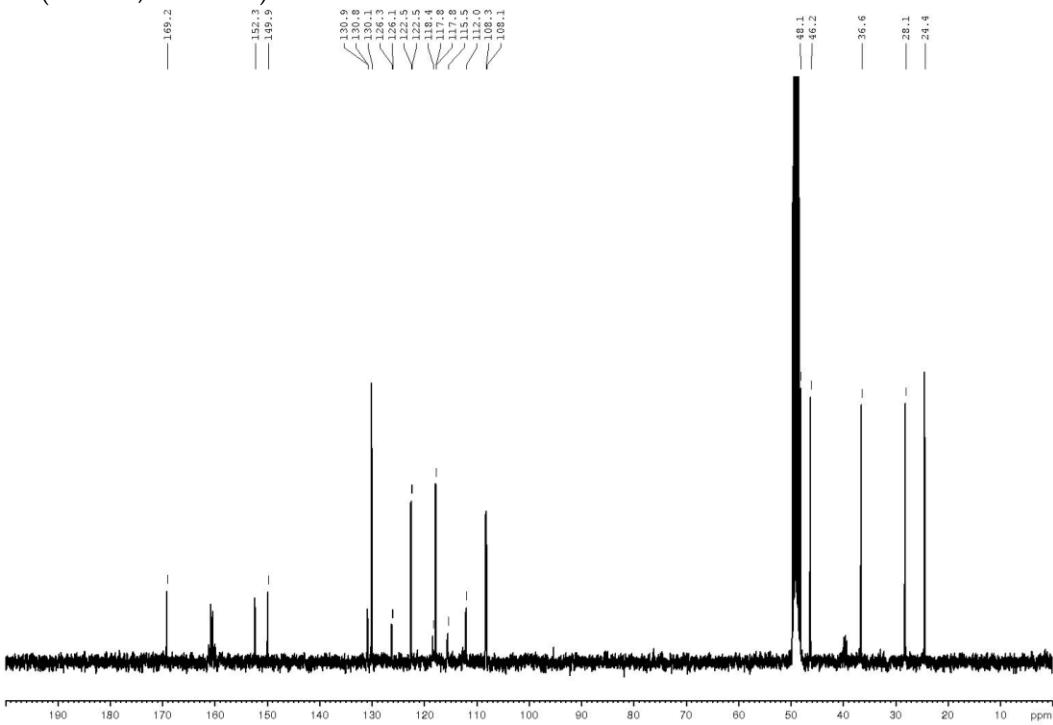
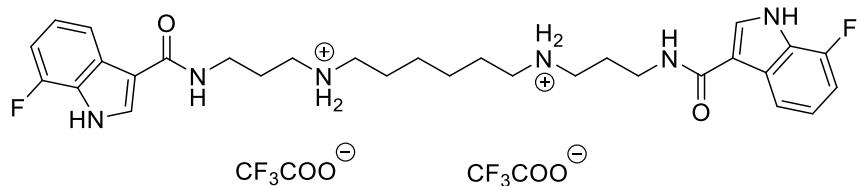
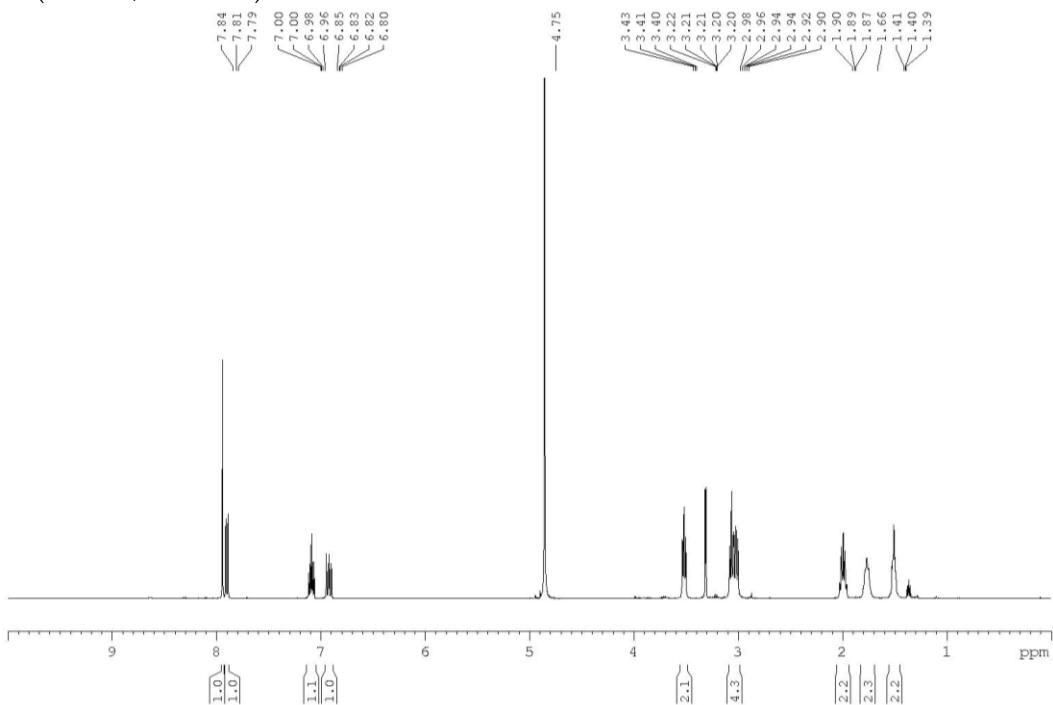


Figure S24 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **16a**



¹H NMR (CD_3OD , 400 MHz):



¹³C NMR (CD_3OD , 100 MHz):

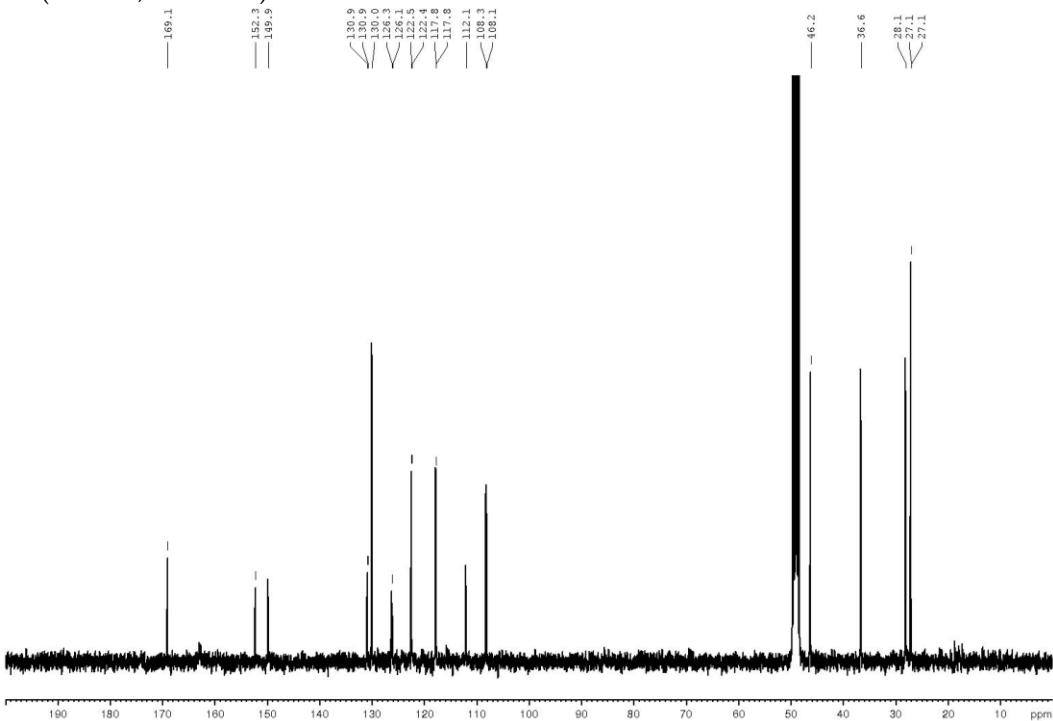
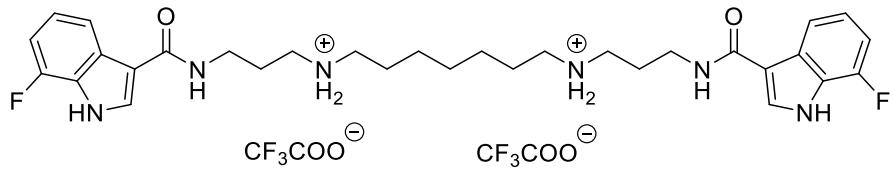
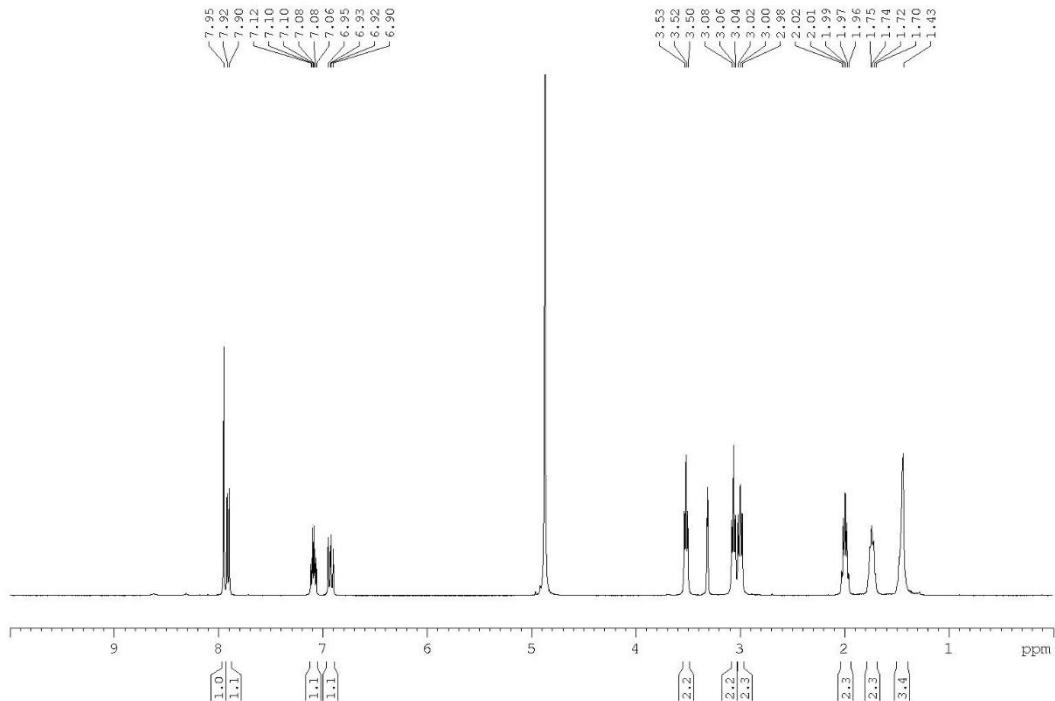


Figure S25 ¹H (CD_3OD , 400 MHz) and ¹³C (CD_3OD , 100 MHz) NMR spectra for **16b**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

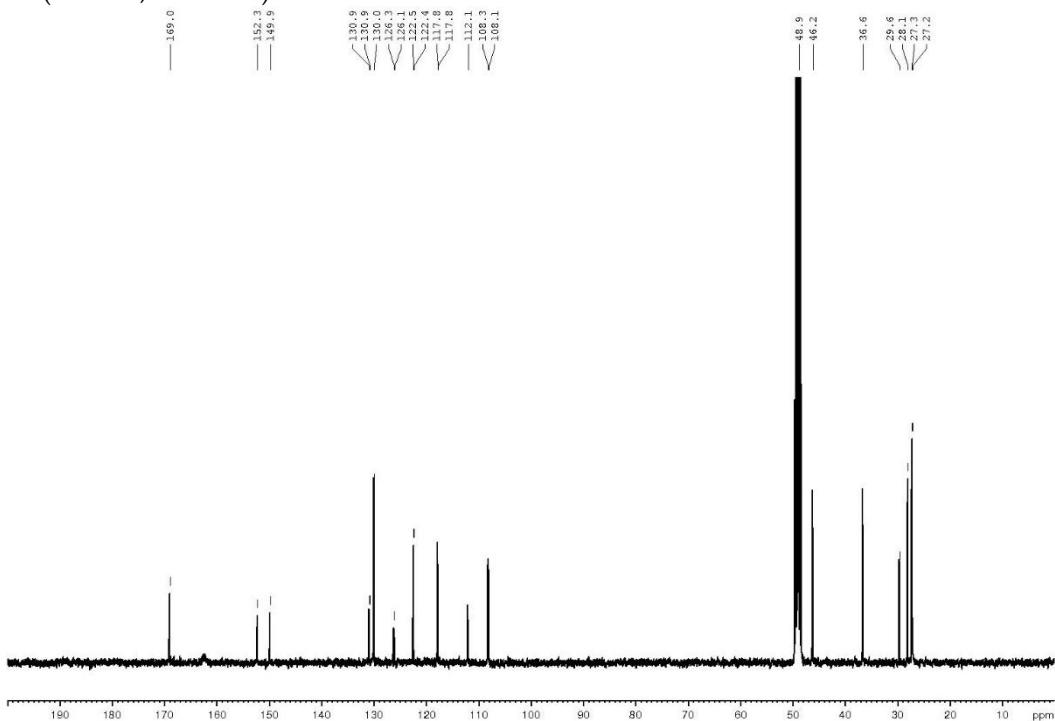
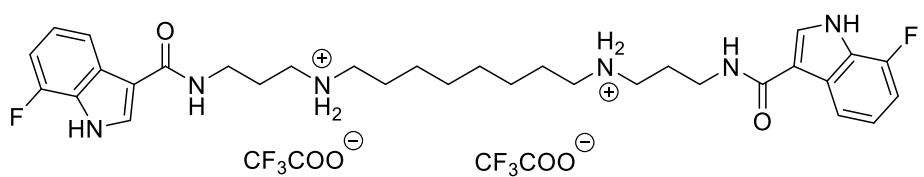
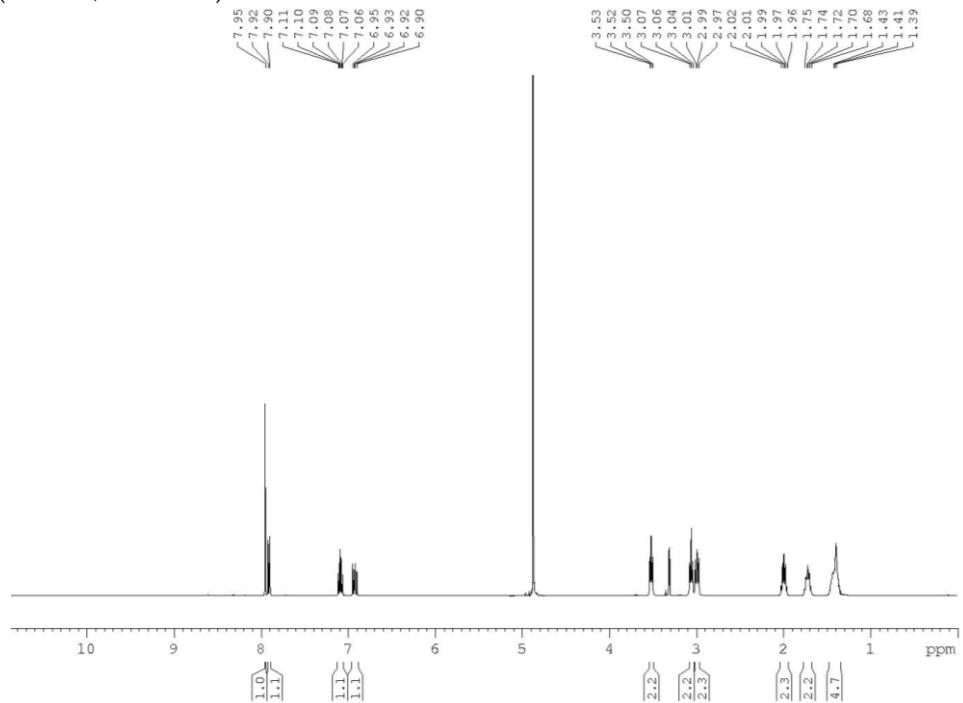


Figure S26 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **16c**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

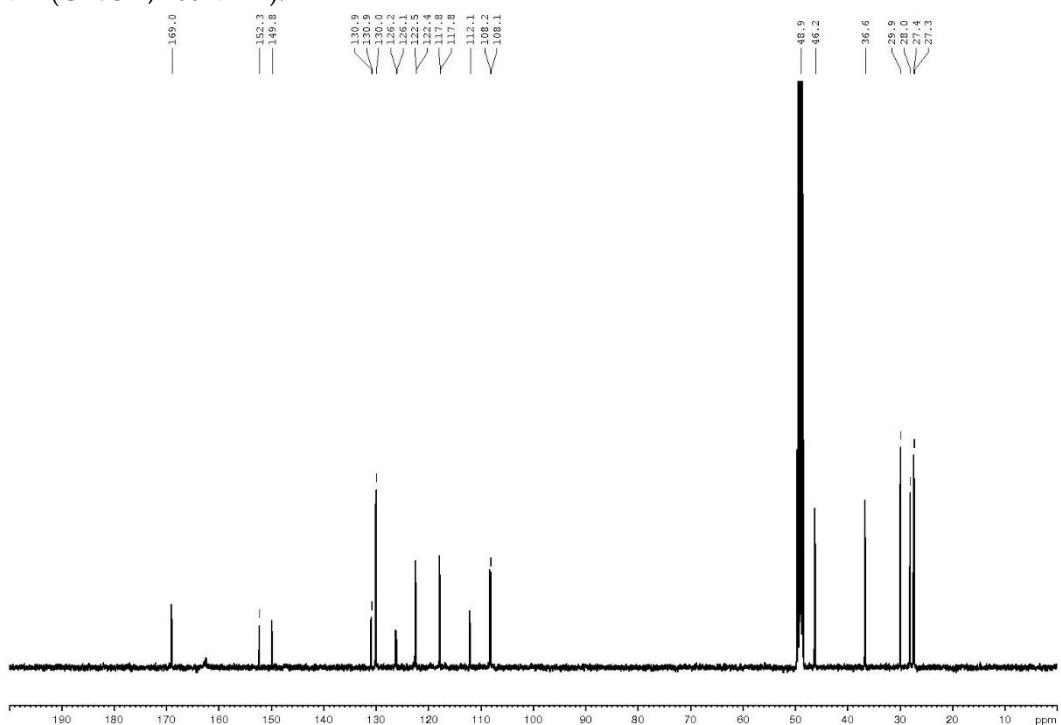
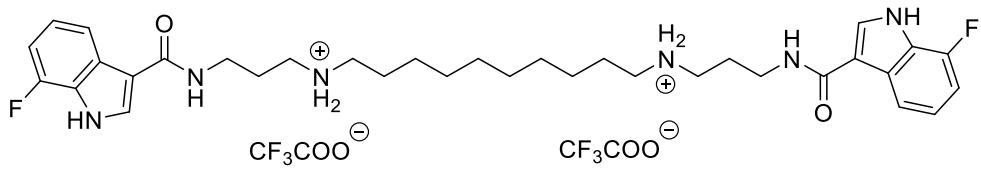
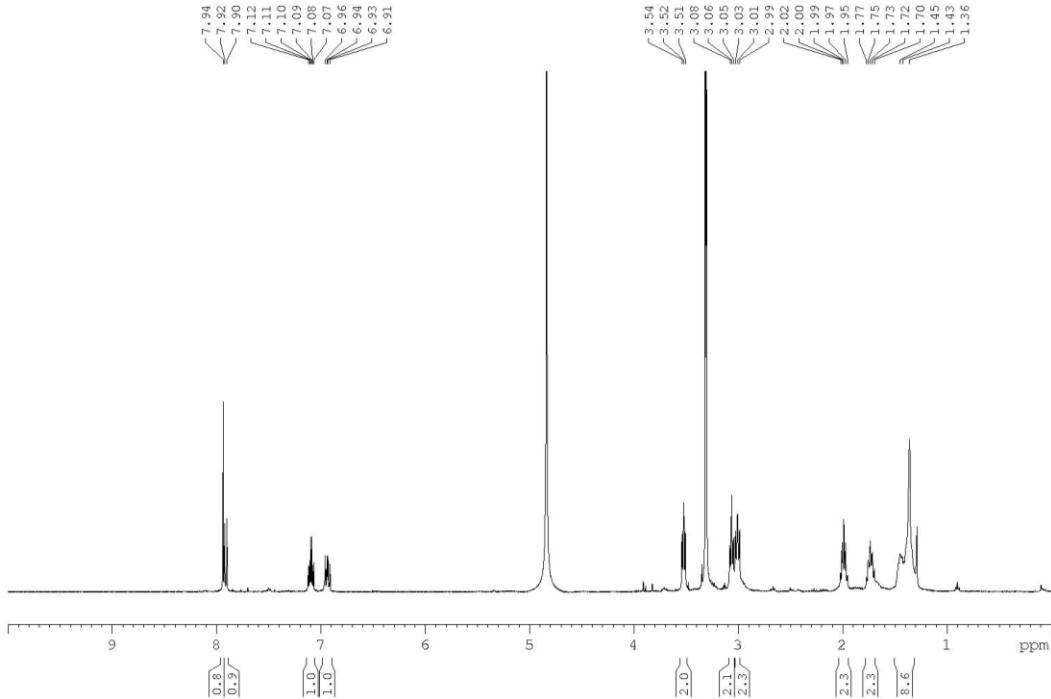


Figure S27 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **16d**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

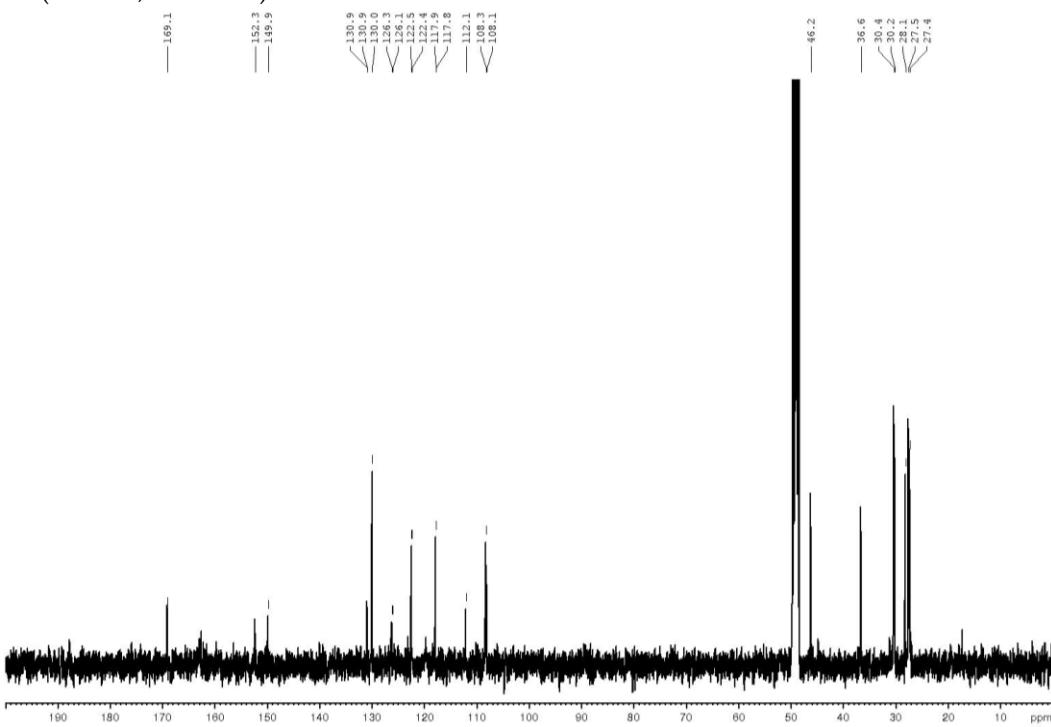
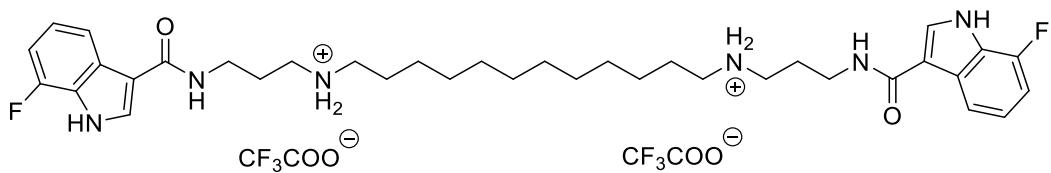
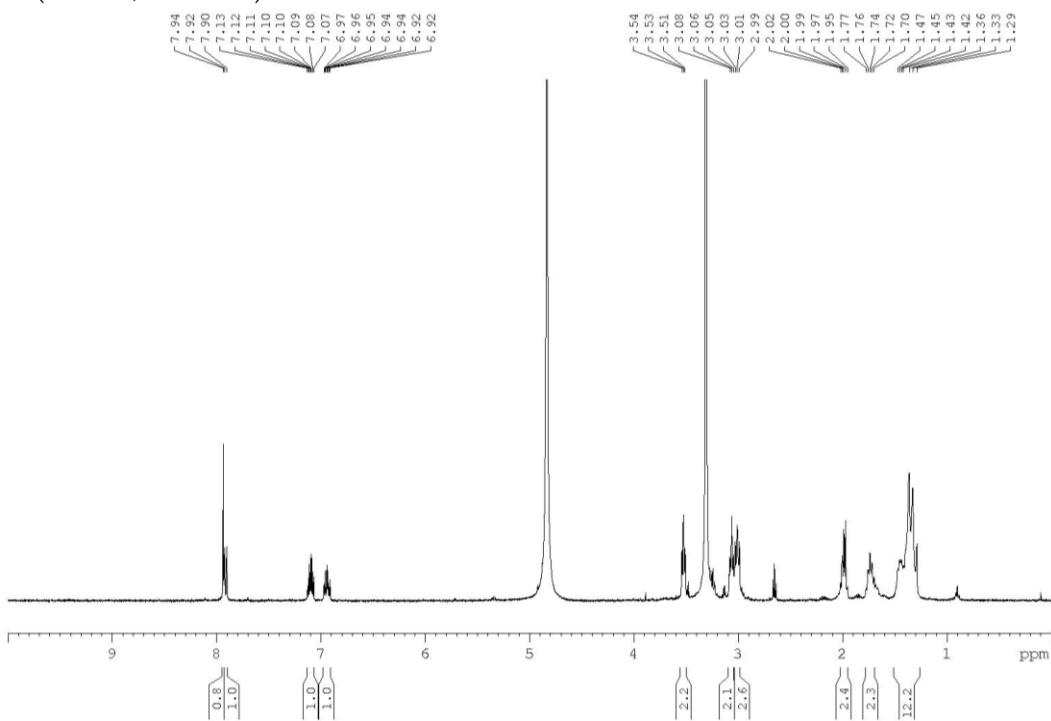


Figure S28 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **16e**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

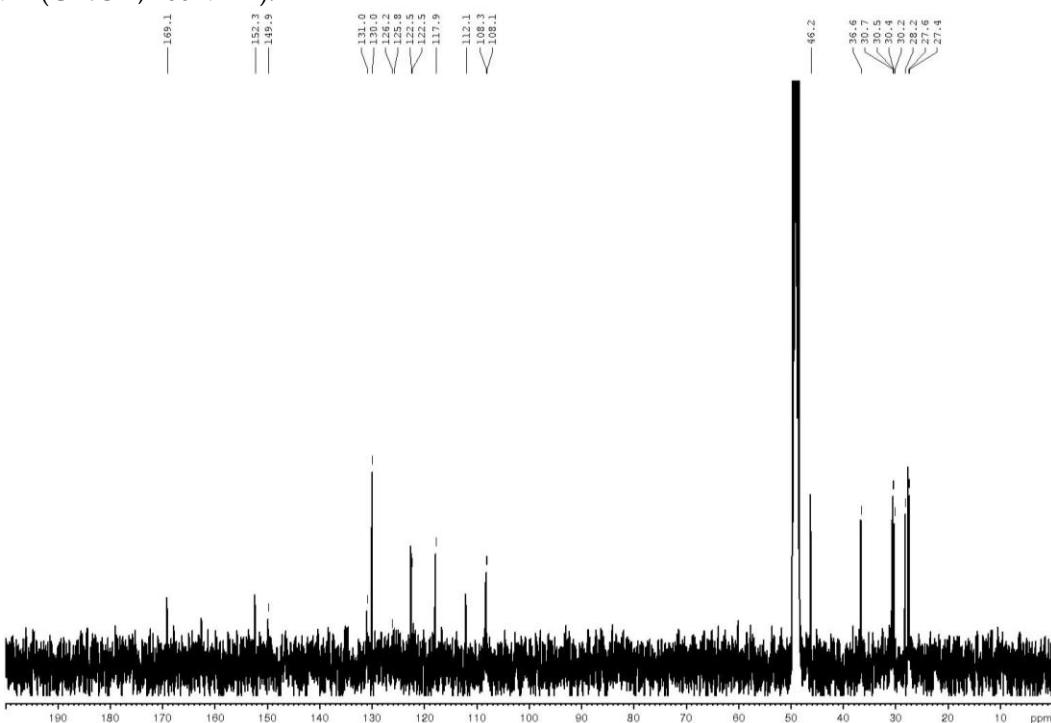
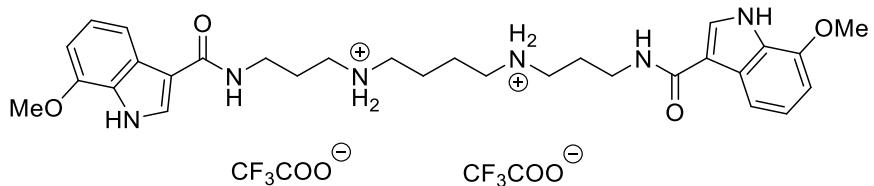


Figure S29 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **16f**



^1H NMR (CD_3OD , 400 MHz):

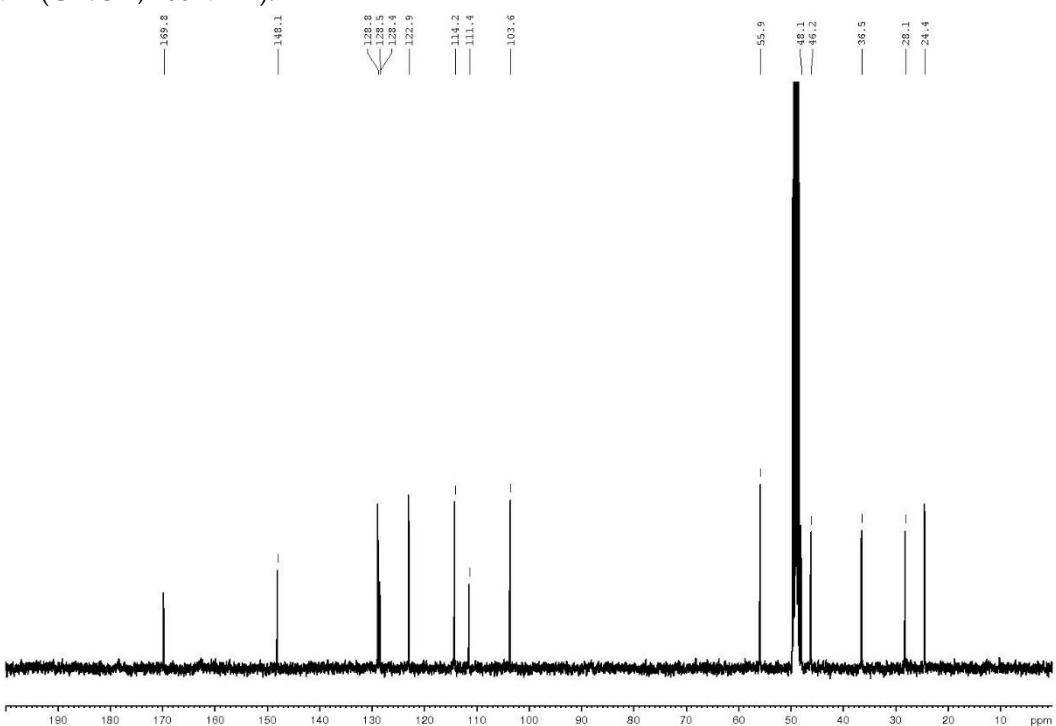
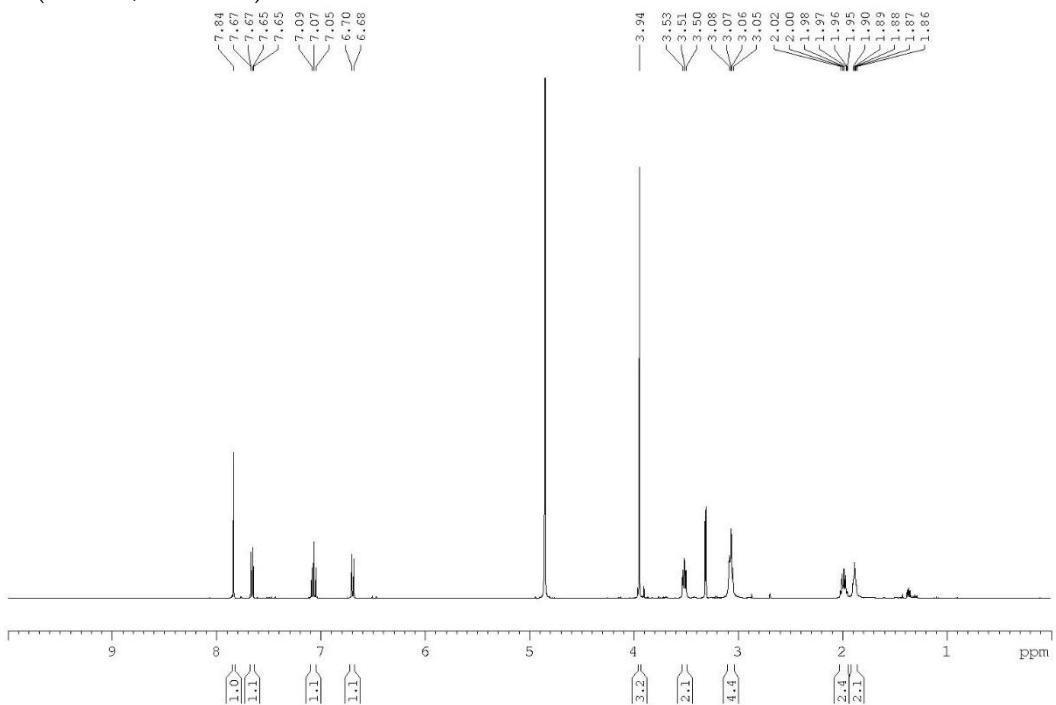
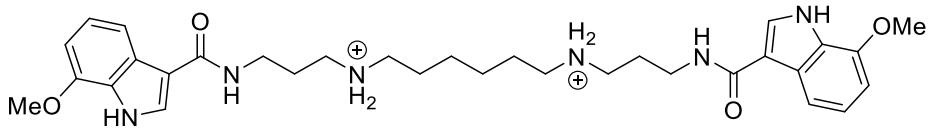
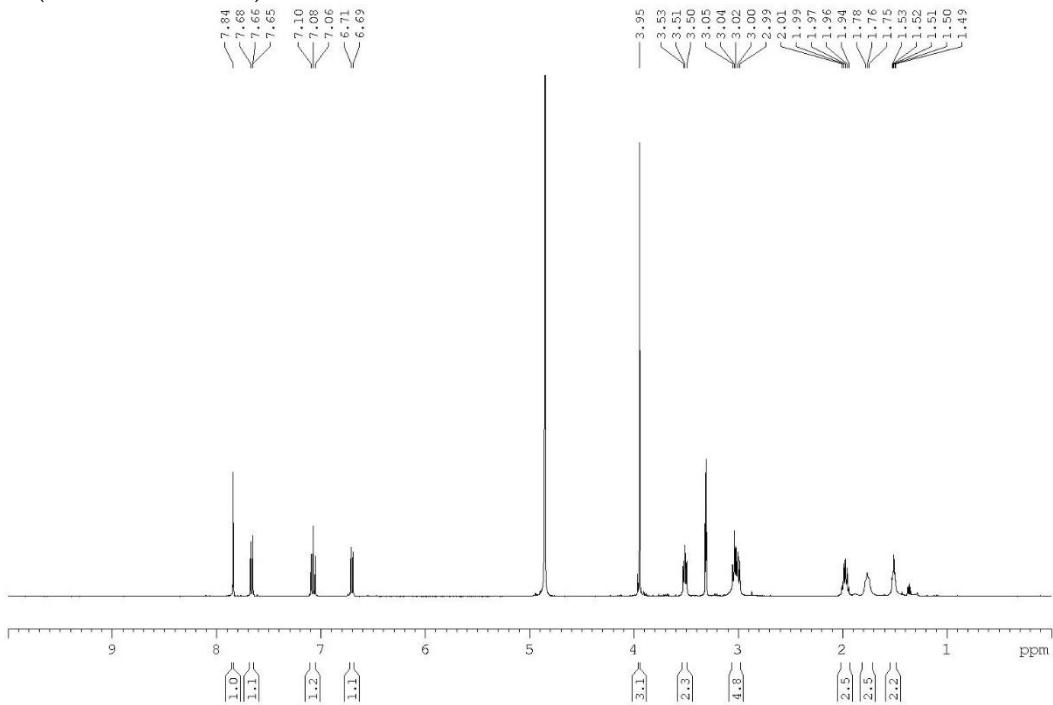


Figure S30 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **17a**



$\text{CF}_3\text{COO}^\ominus$

^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

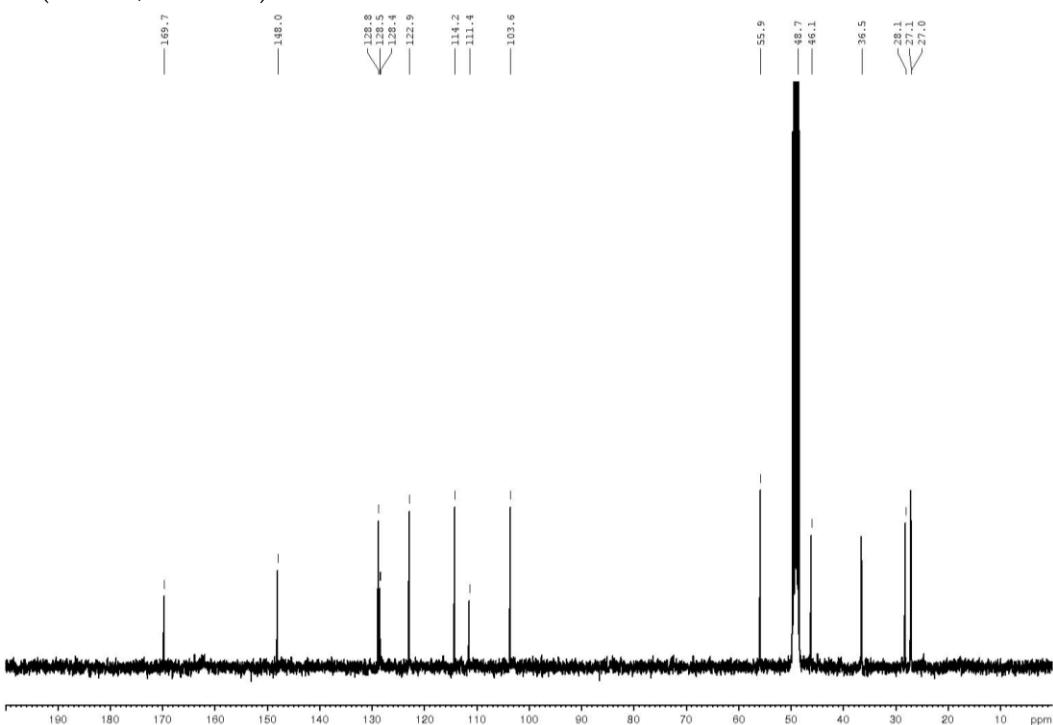
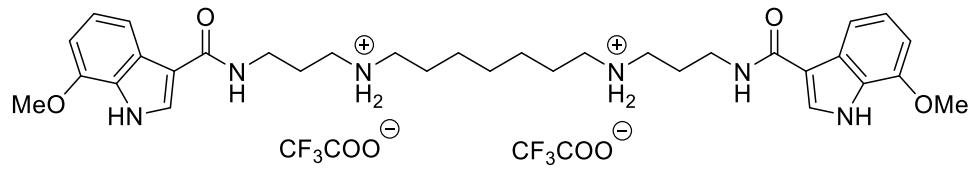
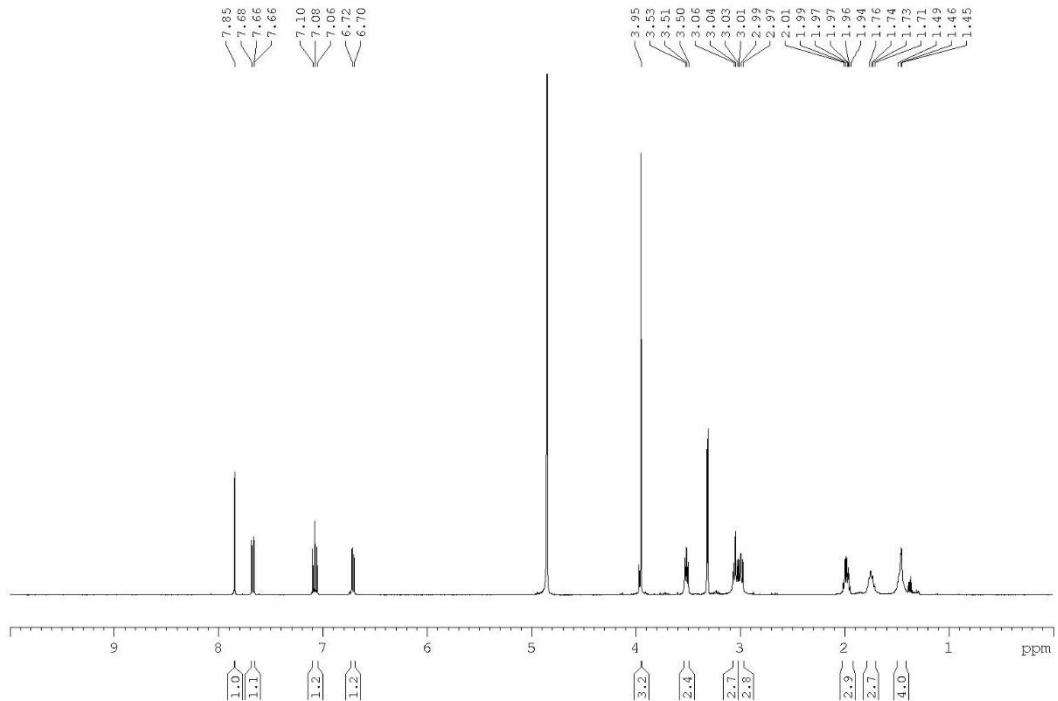


Figure S31 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **17b**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

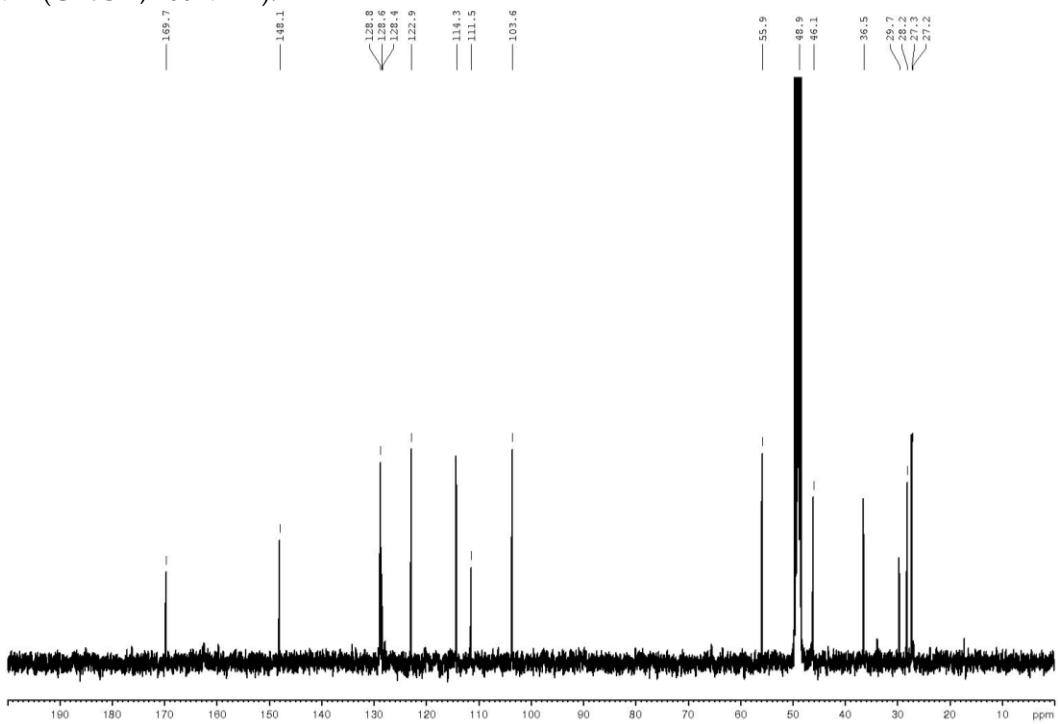
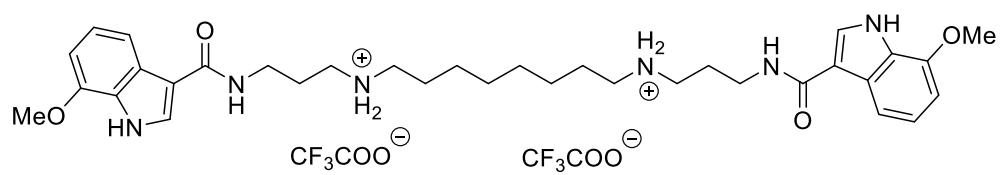
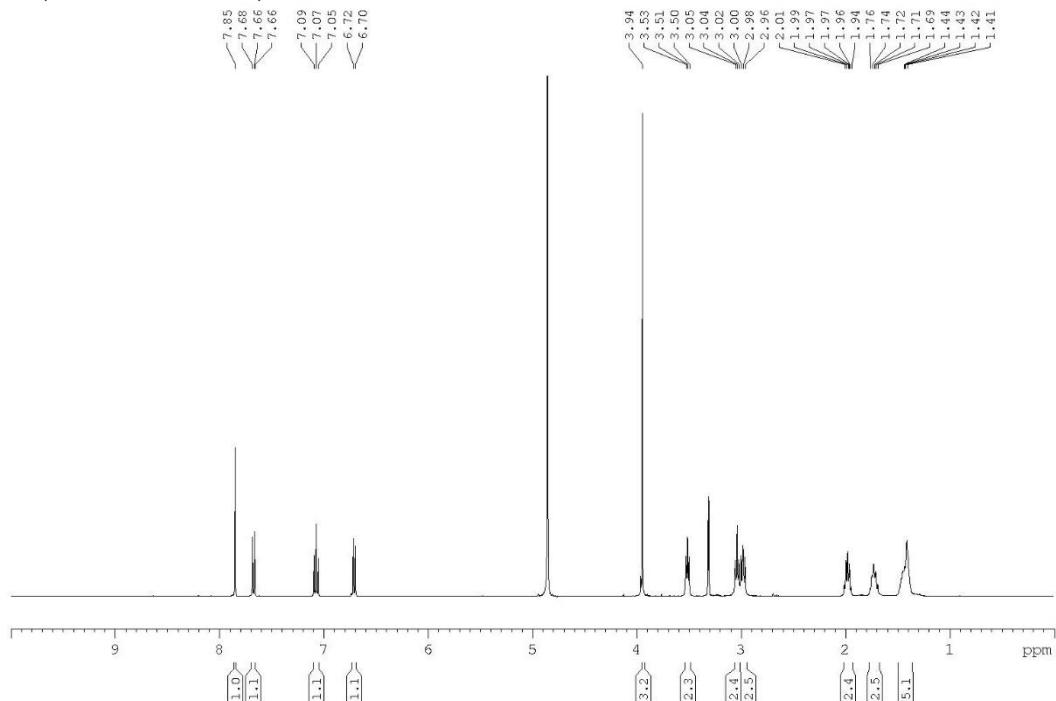


Figure S32 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **17c**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

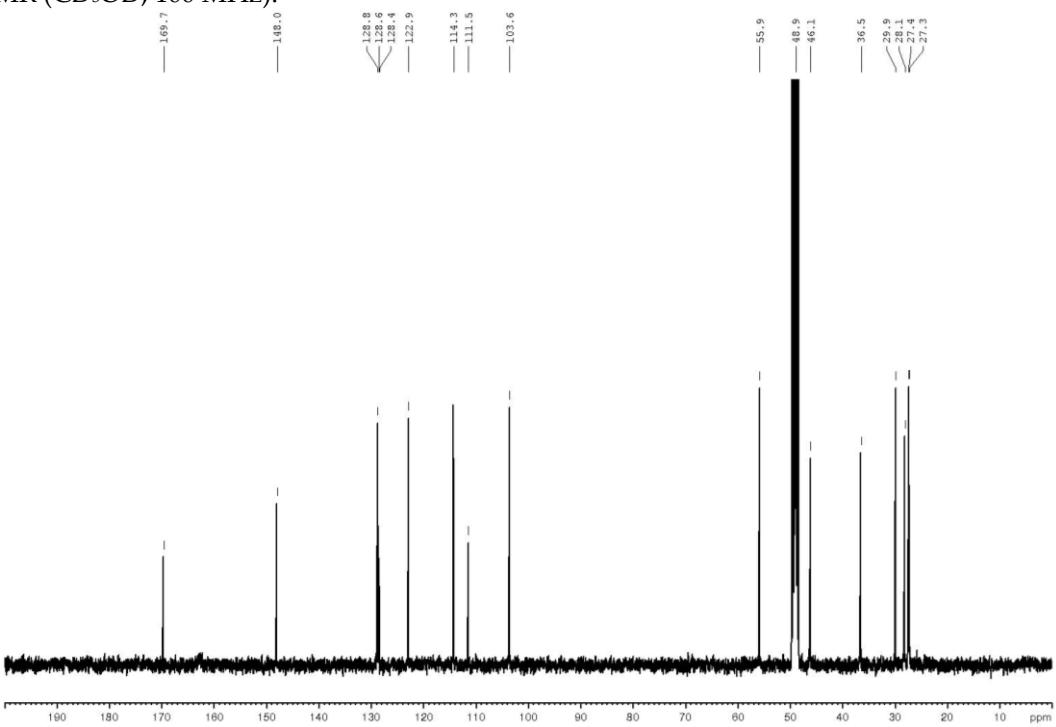
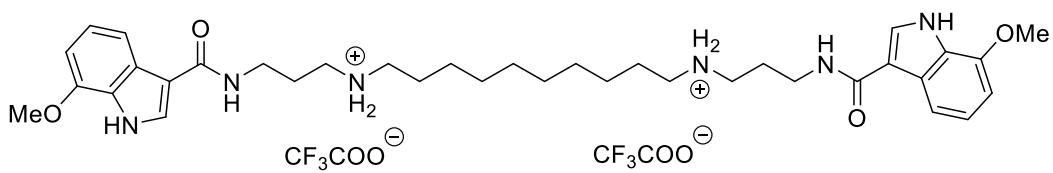
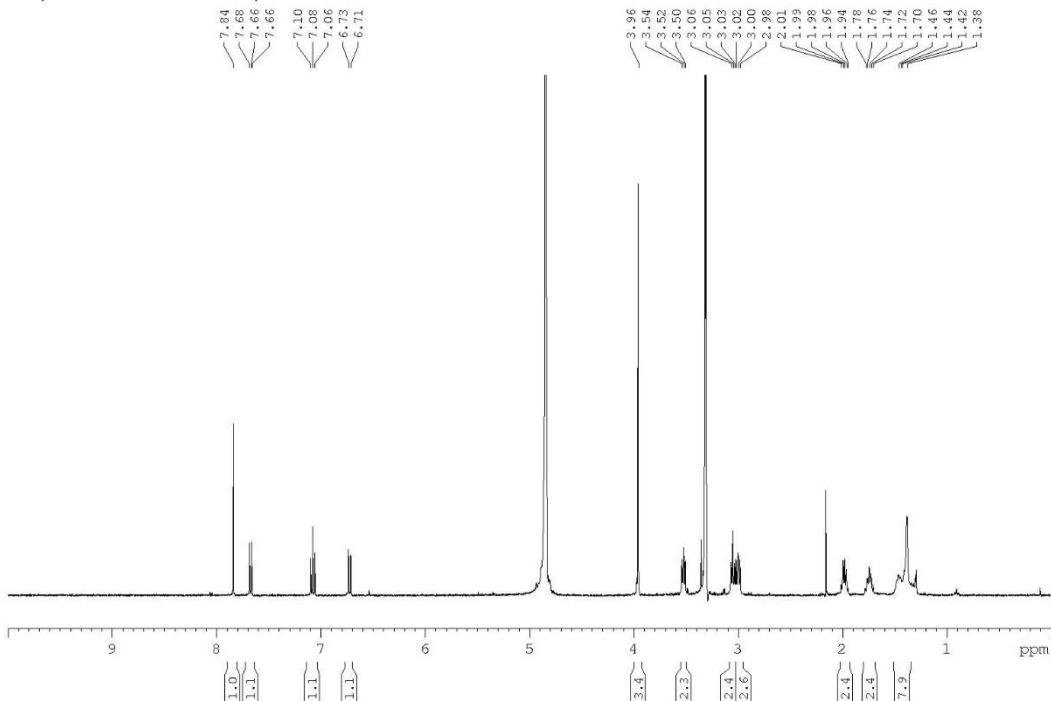


Figure S33 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **17d**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

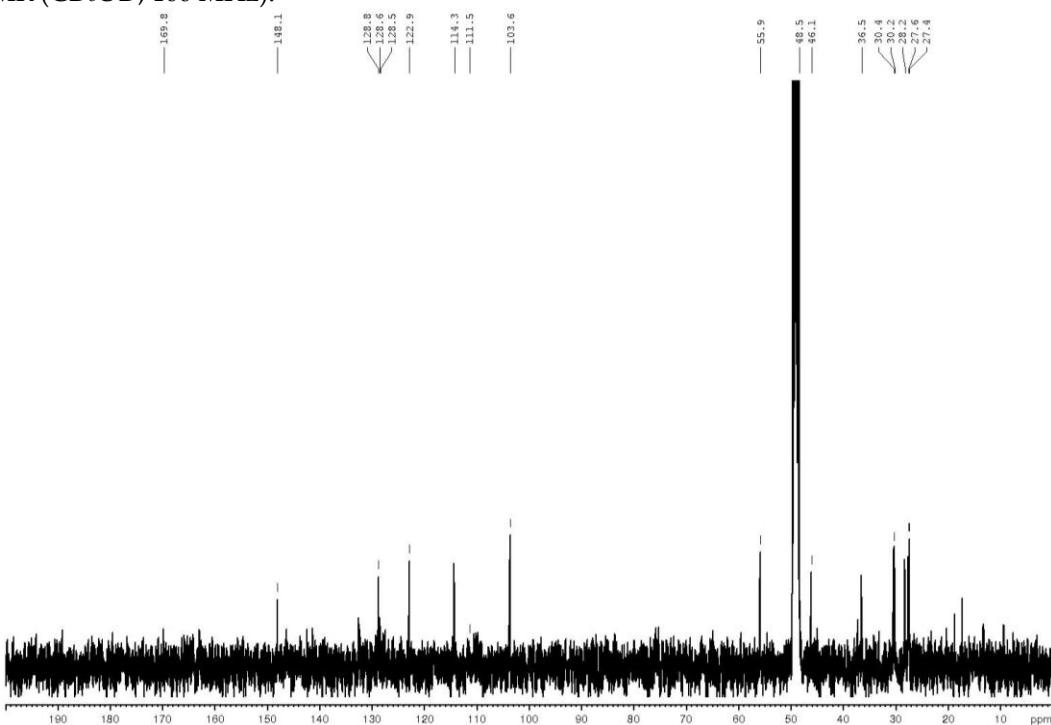
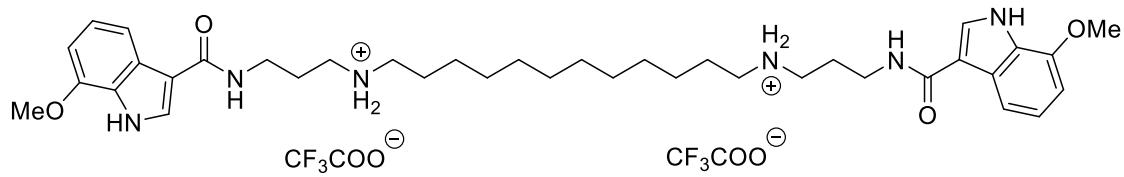
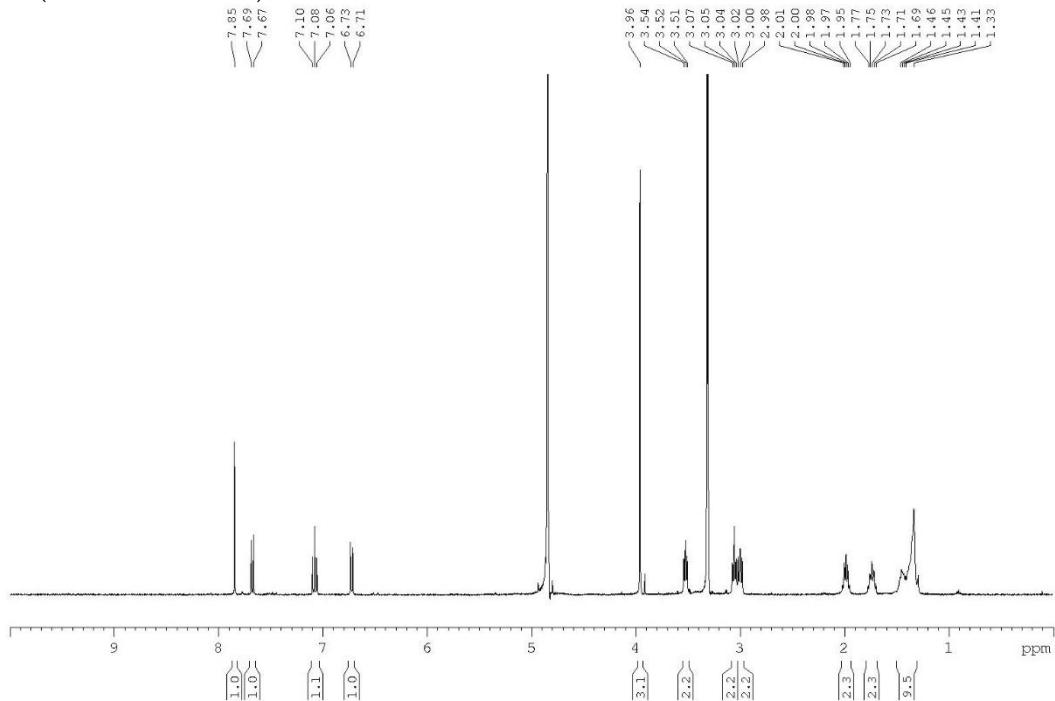


Figure S34 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **17e**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

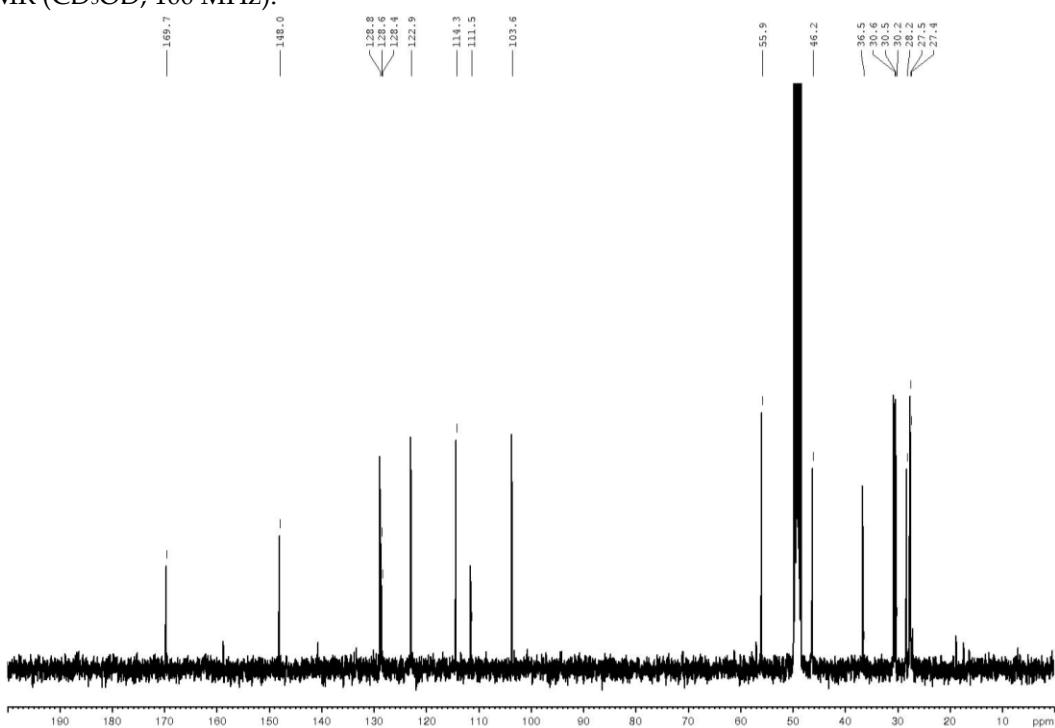
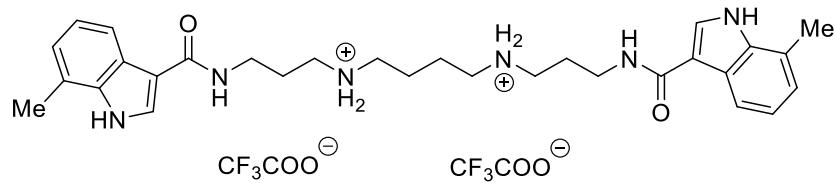
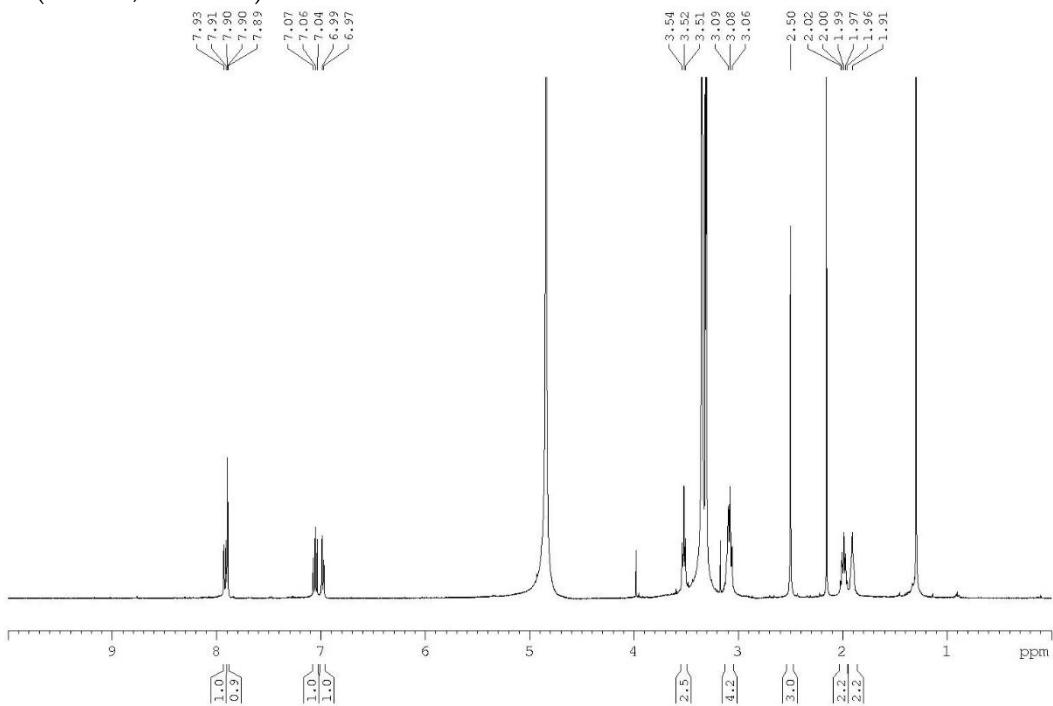


Figure S35 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **17f**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

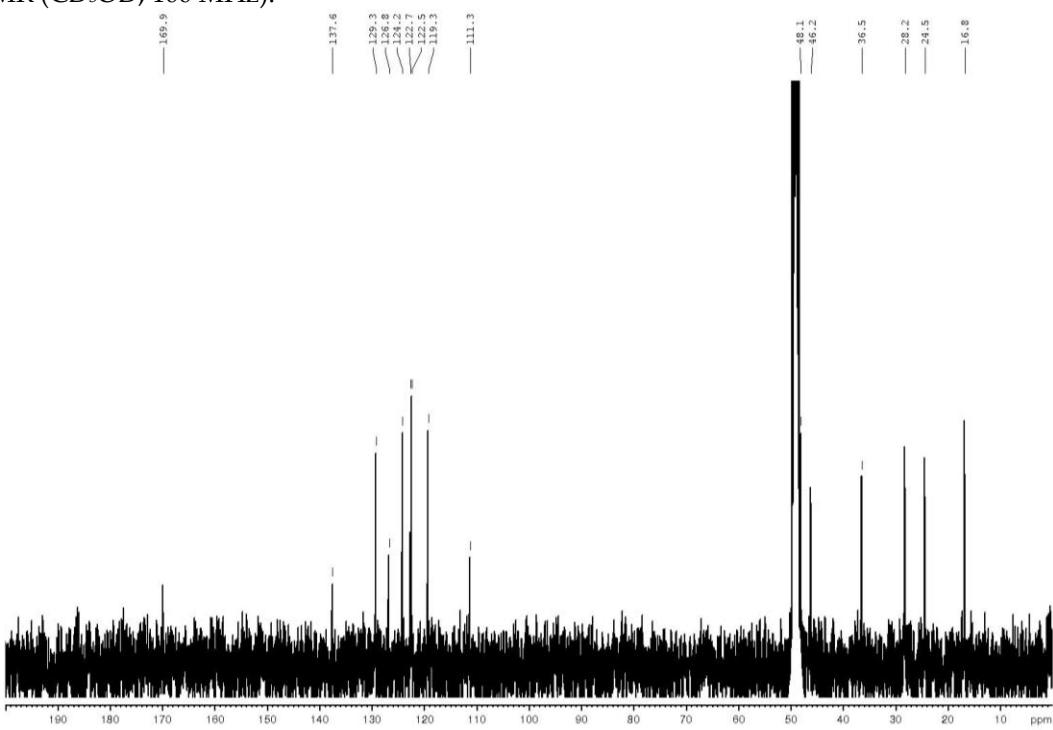
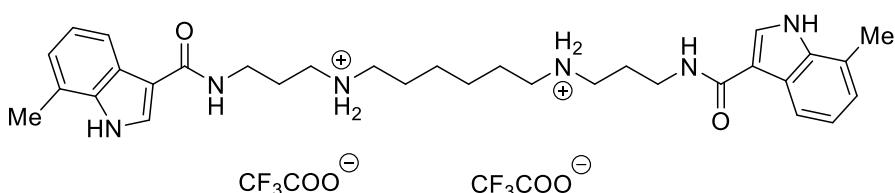
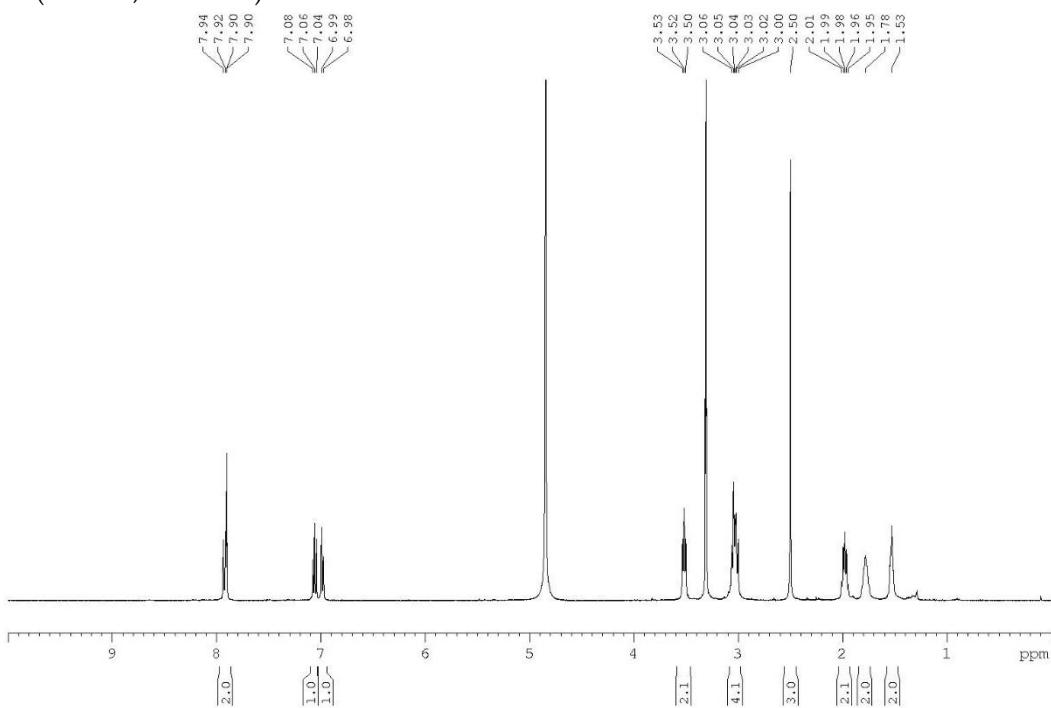


Figure S36 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **18a**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

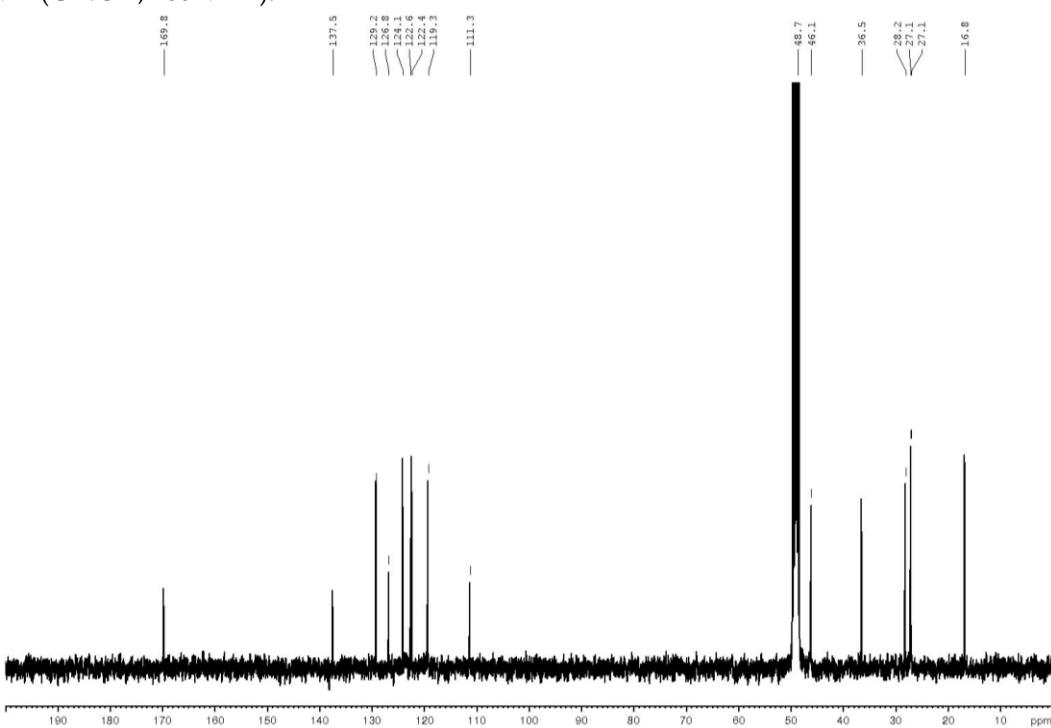
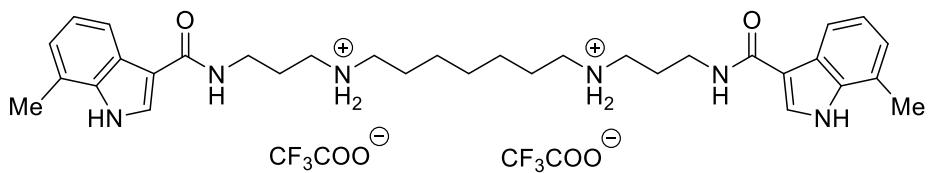
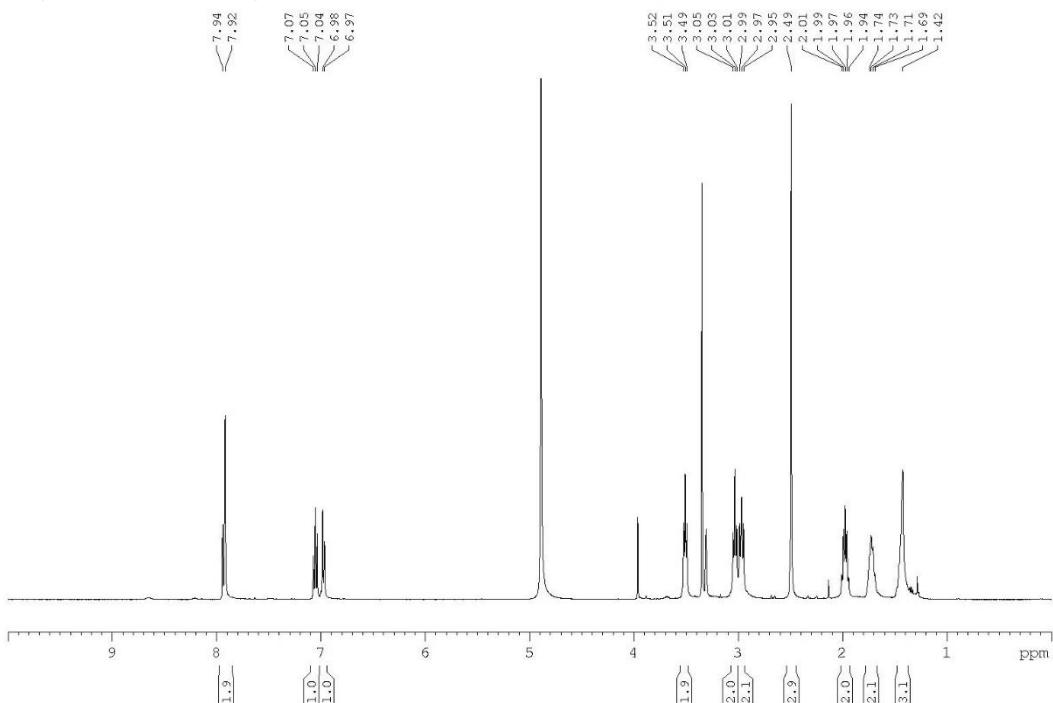


Figure S37 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **18b**



^1H NMR (CD_3OD , 400 MHz):



^{13}C NMR (CD_3OD , 100 MHz):

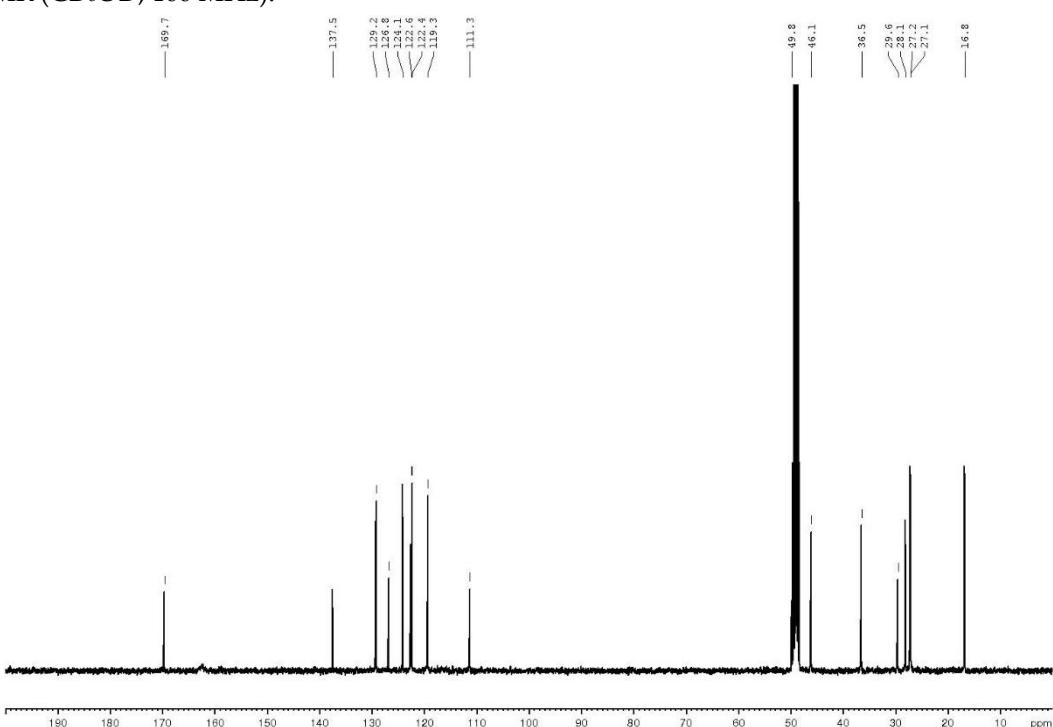
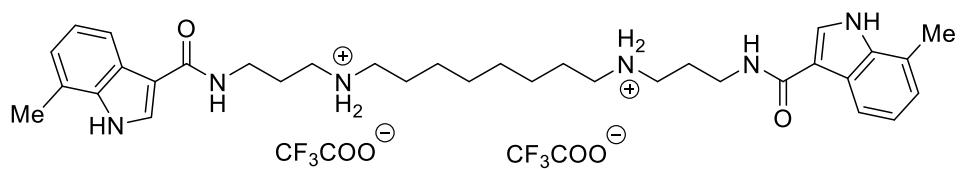
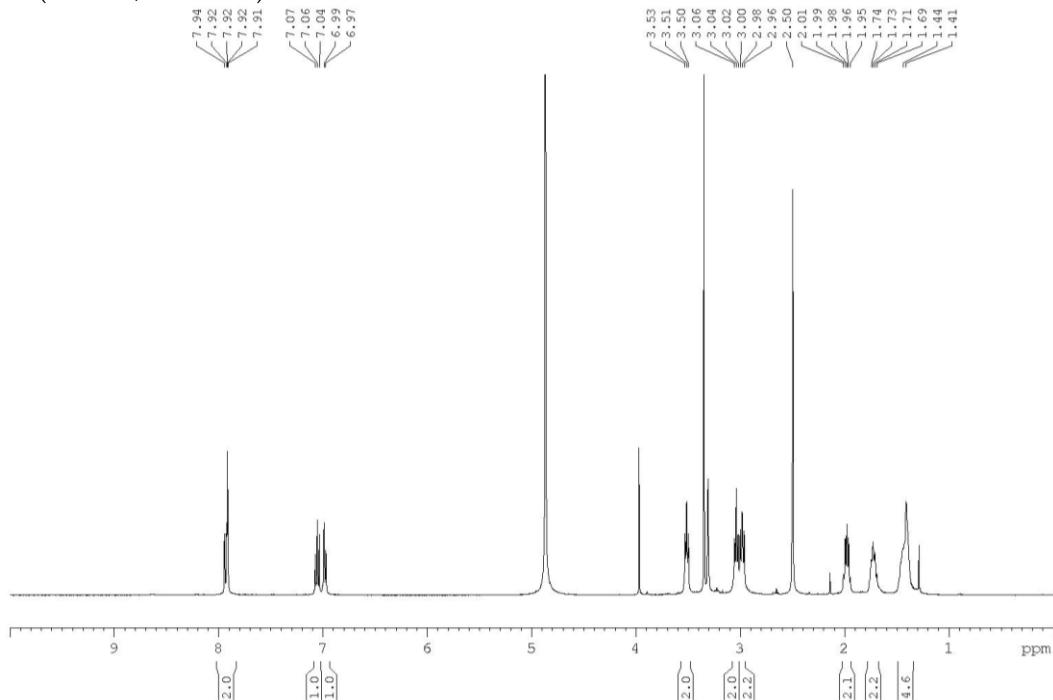


Figure S38 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **18c**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

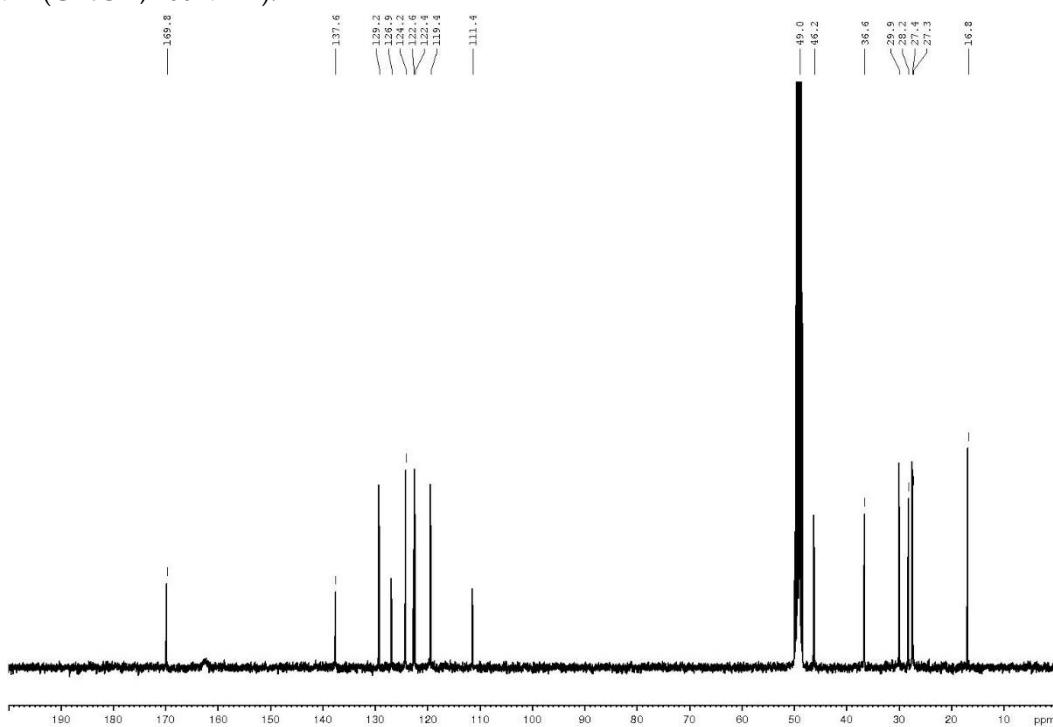
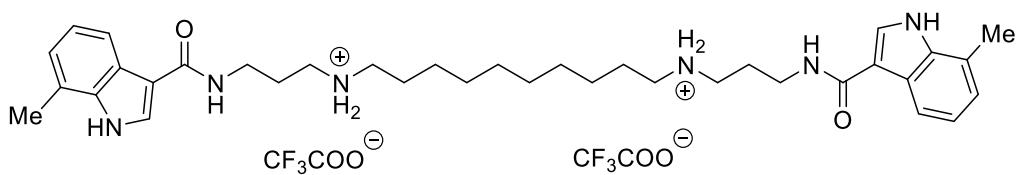
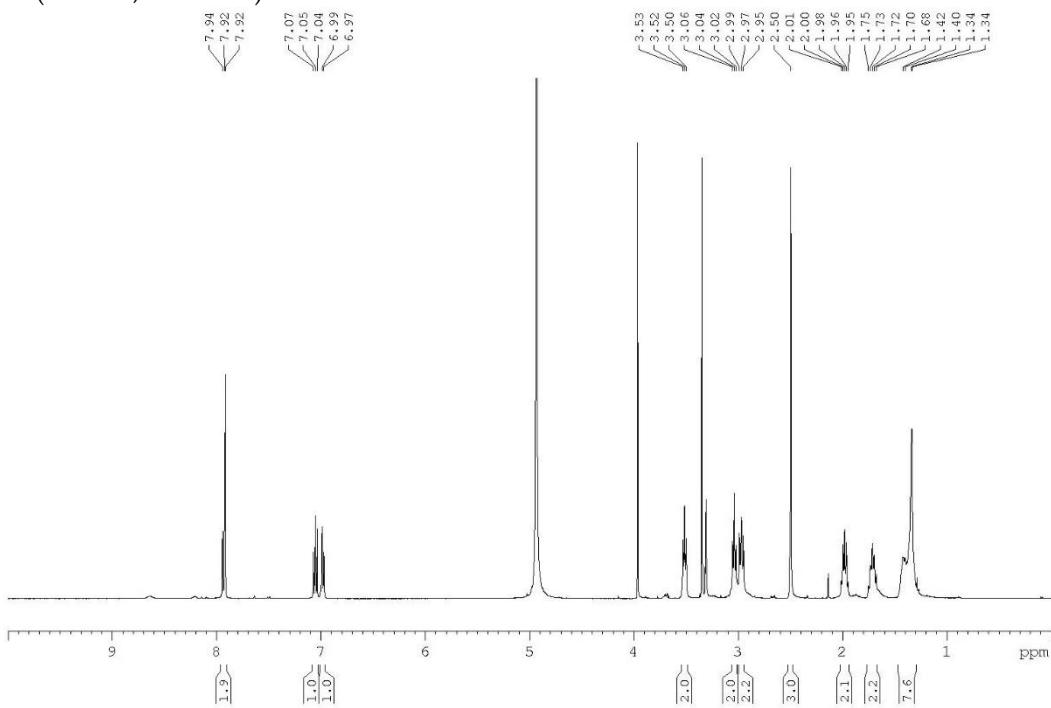


Figure S39 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **18d**



¹H NMR (CD₃OD, 400 MHz):



¹³C NMR (CD₃OD, 100 MHz):

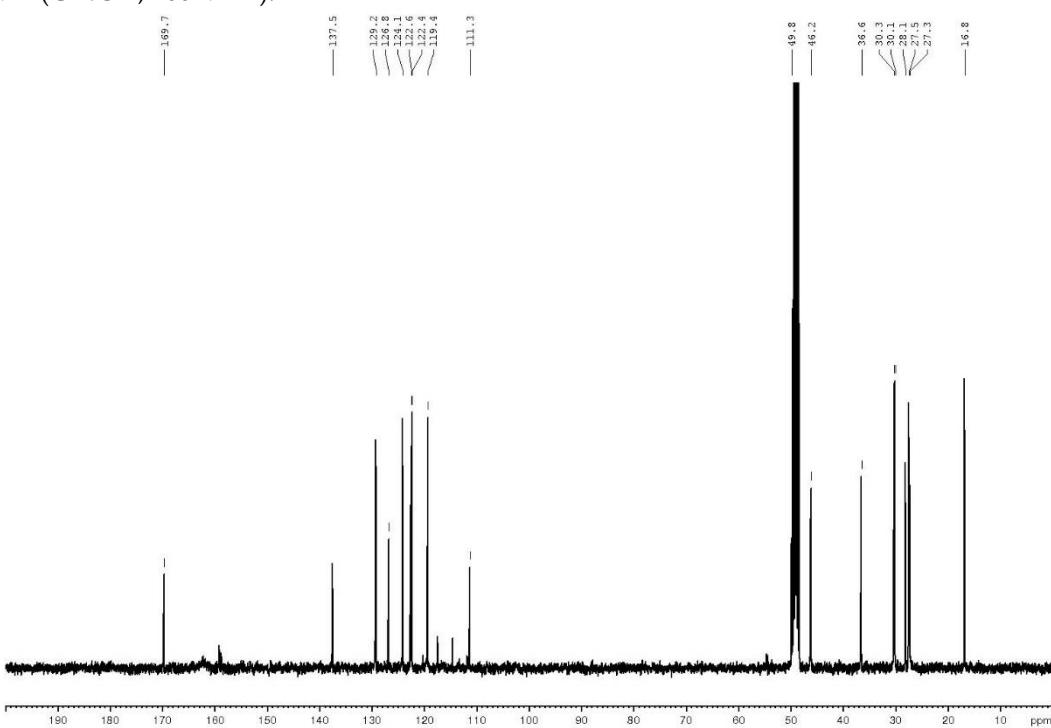
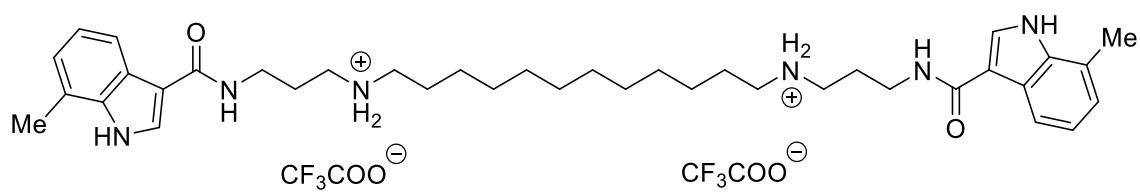


Figure S40 ¹H (CD₃OD, 400 MHz) and ¹³C (CD₃OD, 100 MHz) NMR spectra for **18e**



^1H NMR (CD_3OD , 400 MHz):

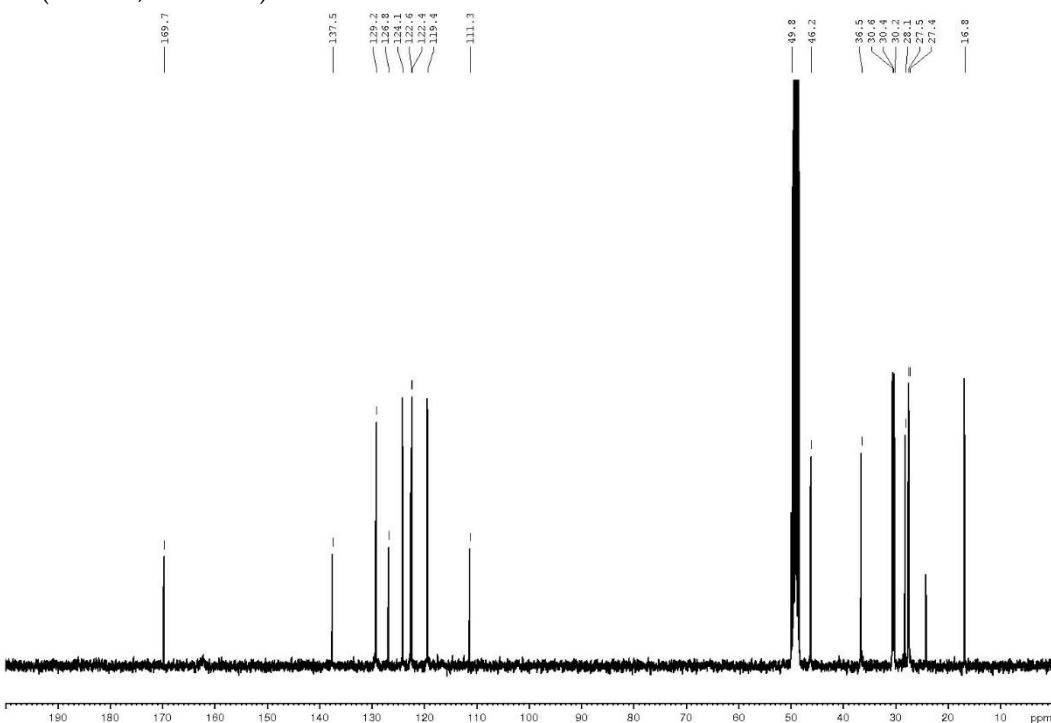
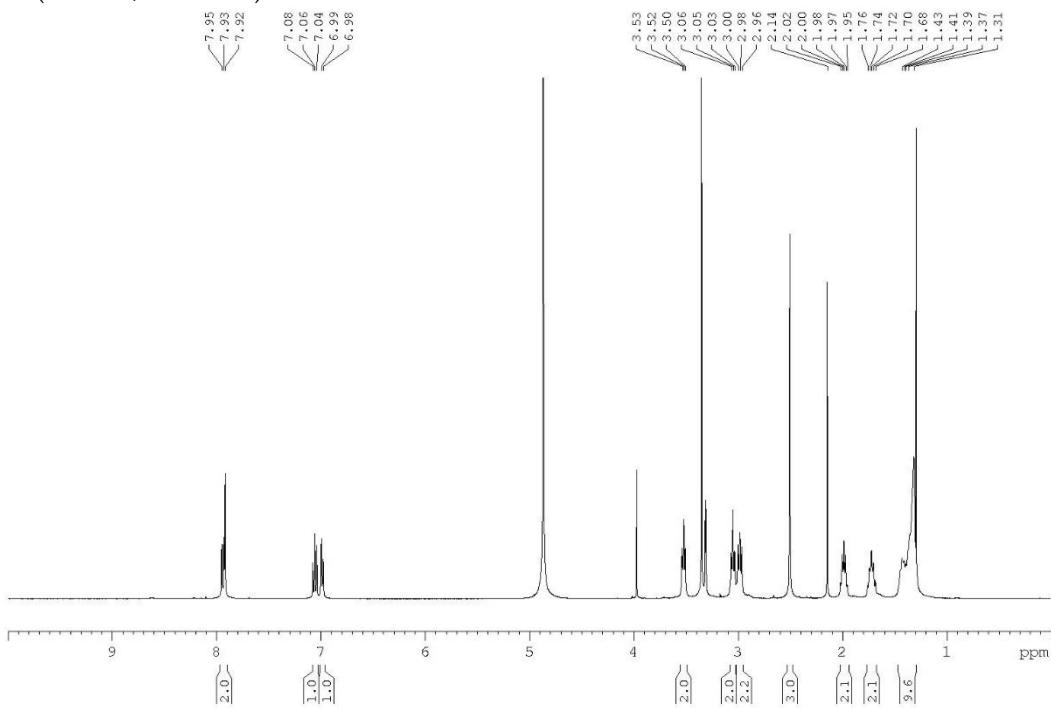


Figure S41 ^1H (CD_3OD , 400 MHz) and ^{13}C (CD_3OD , 100 MHz) NMR spectra for **18f**