

Supporting Information

Investigation of α,ω -disubstituted polyamine-cholic acid conjugates identifies hyodeoxycholic and chenodeoxycholic scaffolds as non-toxic, potent antimicrobials

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

¹ School of Chemical Sciences, The University of Auckland, Private Bag 92019, Auckland 1142, New Zealand; ksue827@aucklanduni.ac.nz (K.S.); m.cadelis@auckland.ac.nz (M.M.C.); b.copp@auckland.ac.nz (B.C)

² UMR MD1 "Membranes et Cibles Thérapeutiques", U1261 INSERM, Faculté de Pharmacie, Aix-Marseille Université, 27 bd Jean Moulin, 13385 Marseille, France; troia.thomas@gmail.com (T.T.); rouv.flo@hotmail.fr (F.R.); jean-michel.brunel@inserm.fr (J.M.B.)

³ 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; marie-lise.bourguet@mnhn.fr (M-L.B-K)

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

Contents

| | |
|--|-----|
| Figure S1 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 7a . | S2 |
| Figure S2 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 7b . | S3 |
| Figure S3 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 7c . | S4 |
| Figure S4 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 7d . | S5 |
| Figure S5 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 7e . | S6 |
| Figure S6 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 7f . | S7 |
| Figure S7 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 8a . | S8 |
| Figure S8 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 8b . | S9 |
| Figure S9 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 8c . | S10 |
| Figure S10 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 8d . | S11 |
| Figure S11 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 8e . | S12 |
| Figure S12 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 8f . | S13 |
| Figure S13 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for 9a . | S14 |

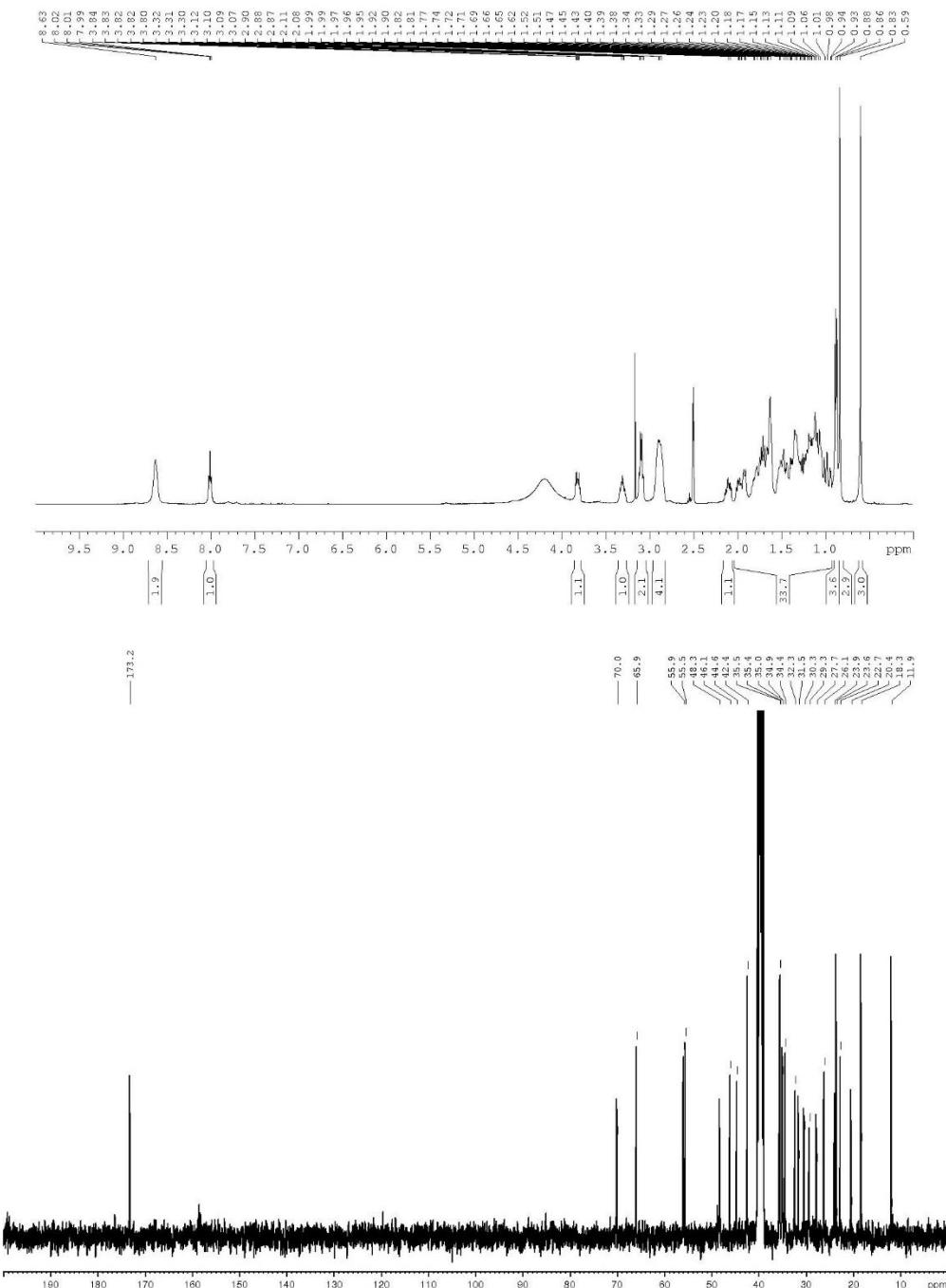
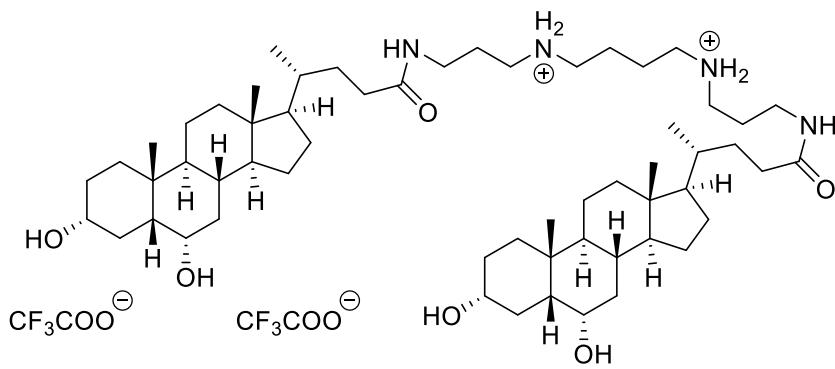


Figure S1 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **7a**.

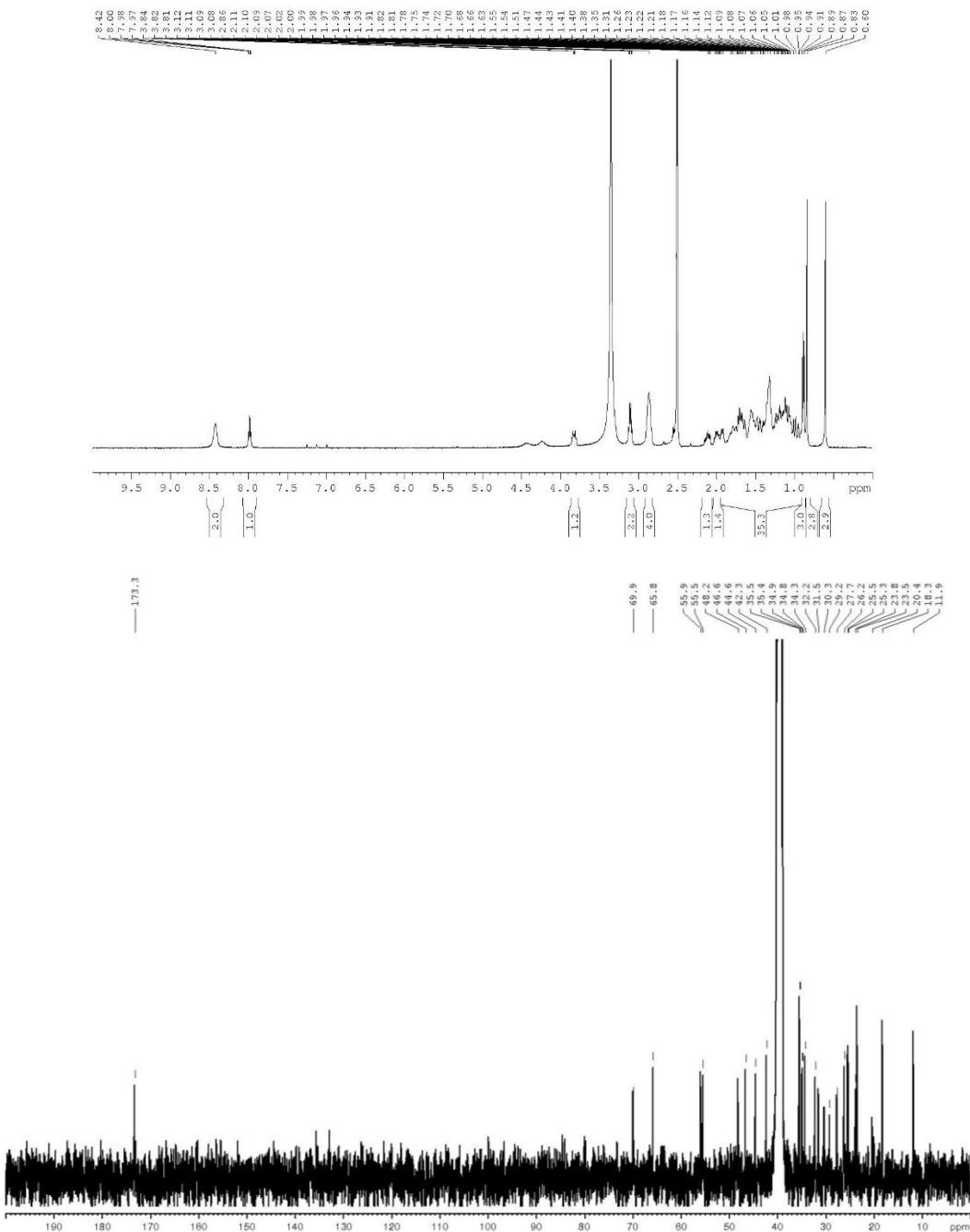
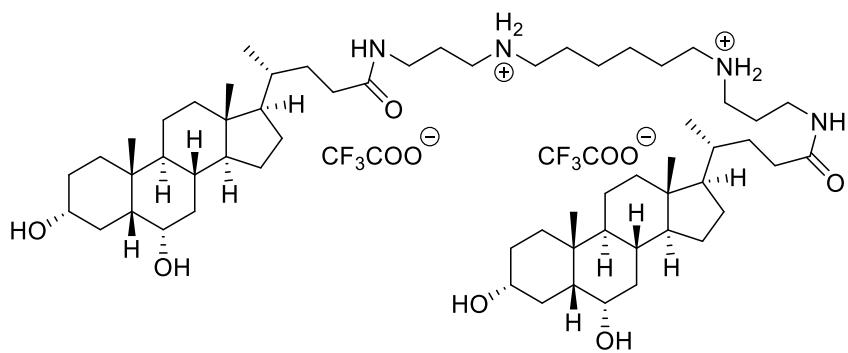


Figure S2 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **7b**.

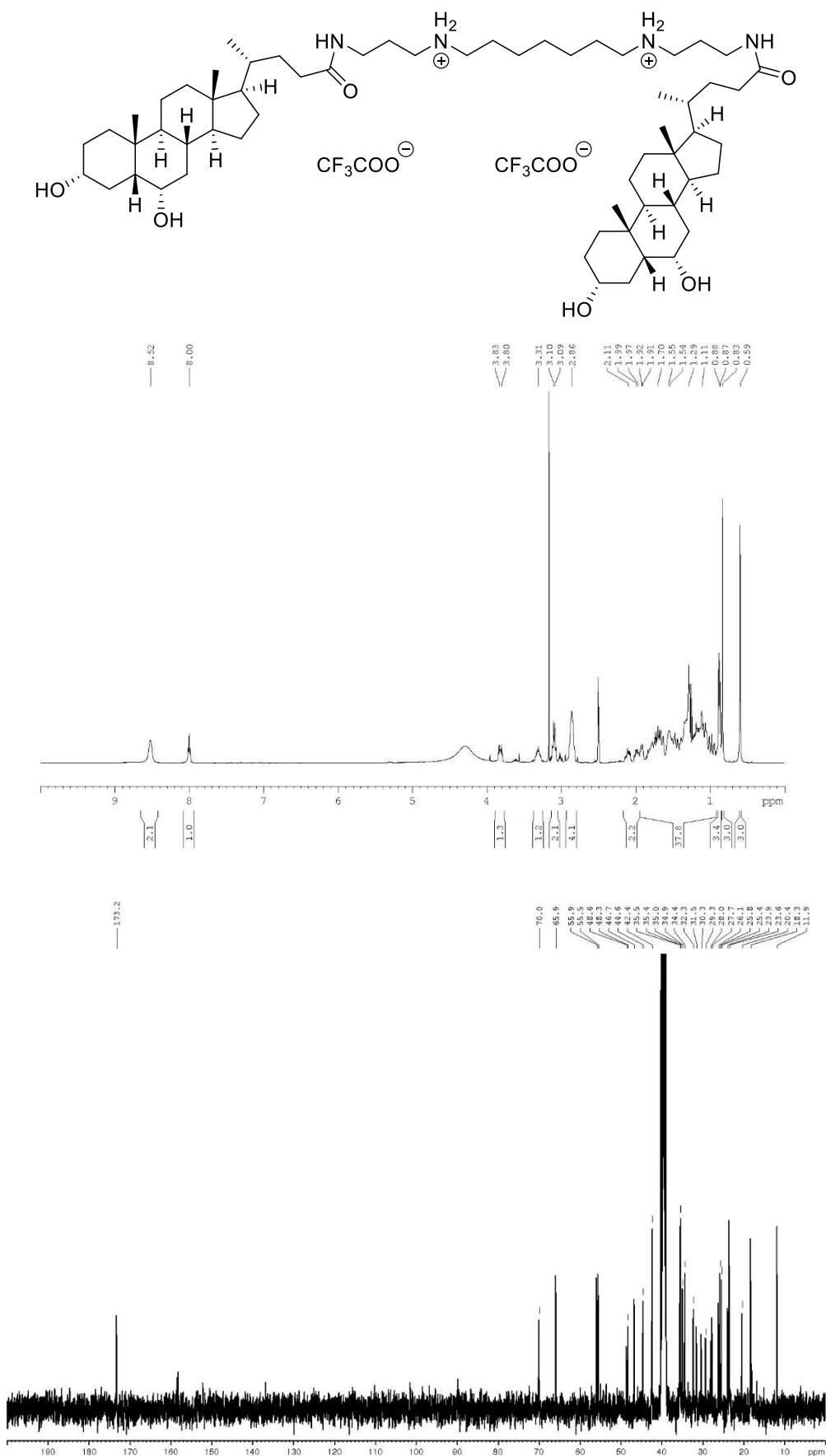


Figure S3 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **7c**.

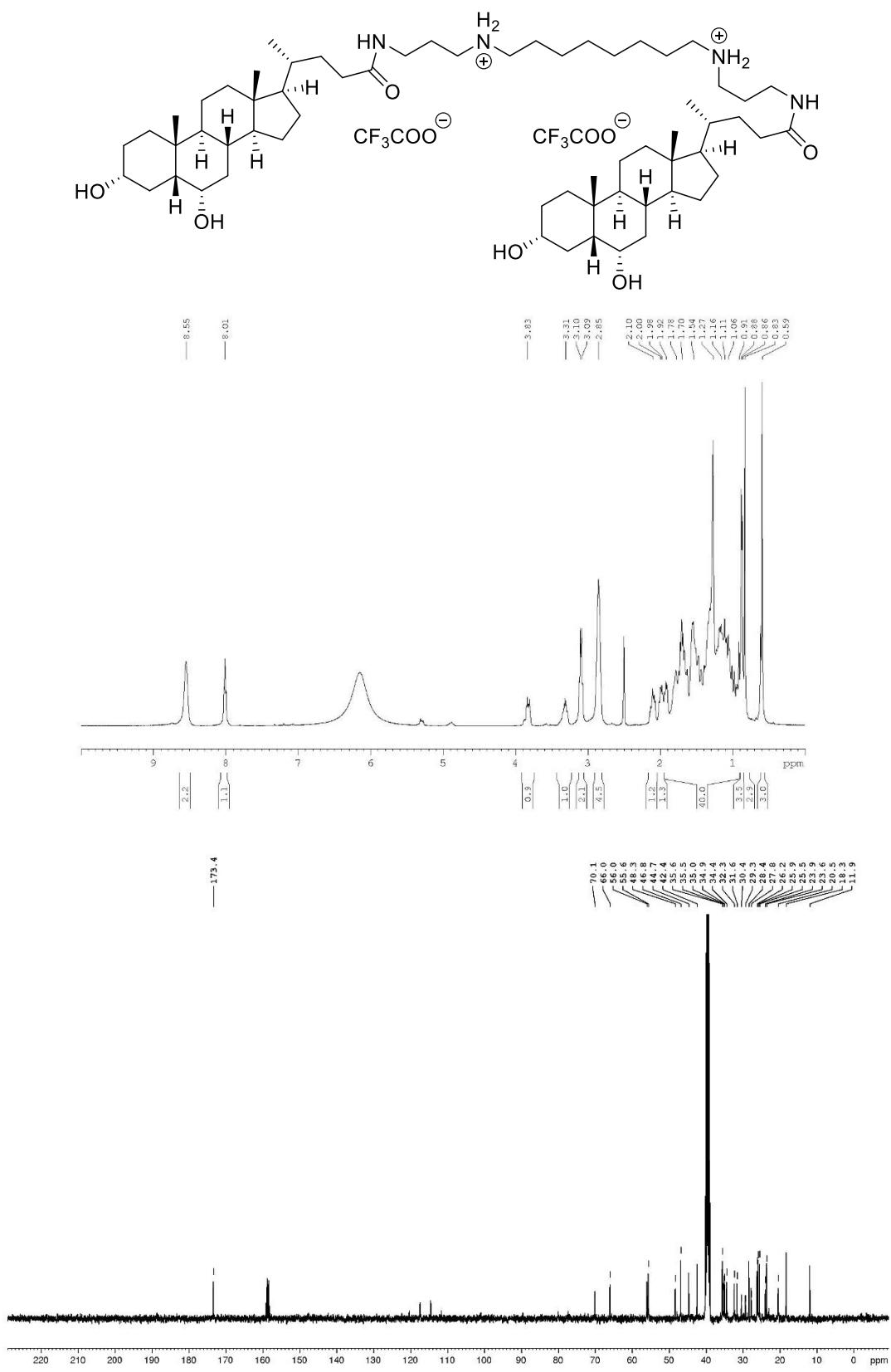


Figure S4 ¹H (DMSO-*d*₆, 400 MHz) and ¹³C (DMSO-*d*₆, 100 MHz) NMR spectra for **7d**.

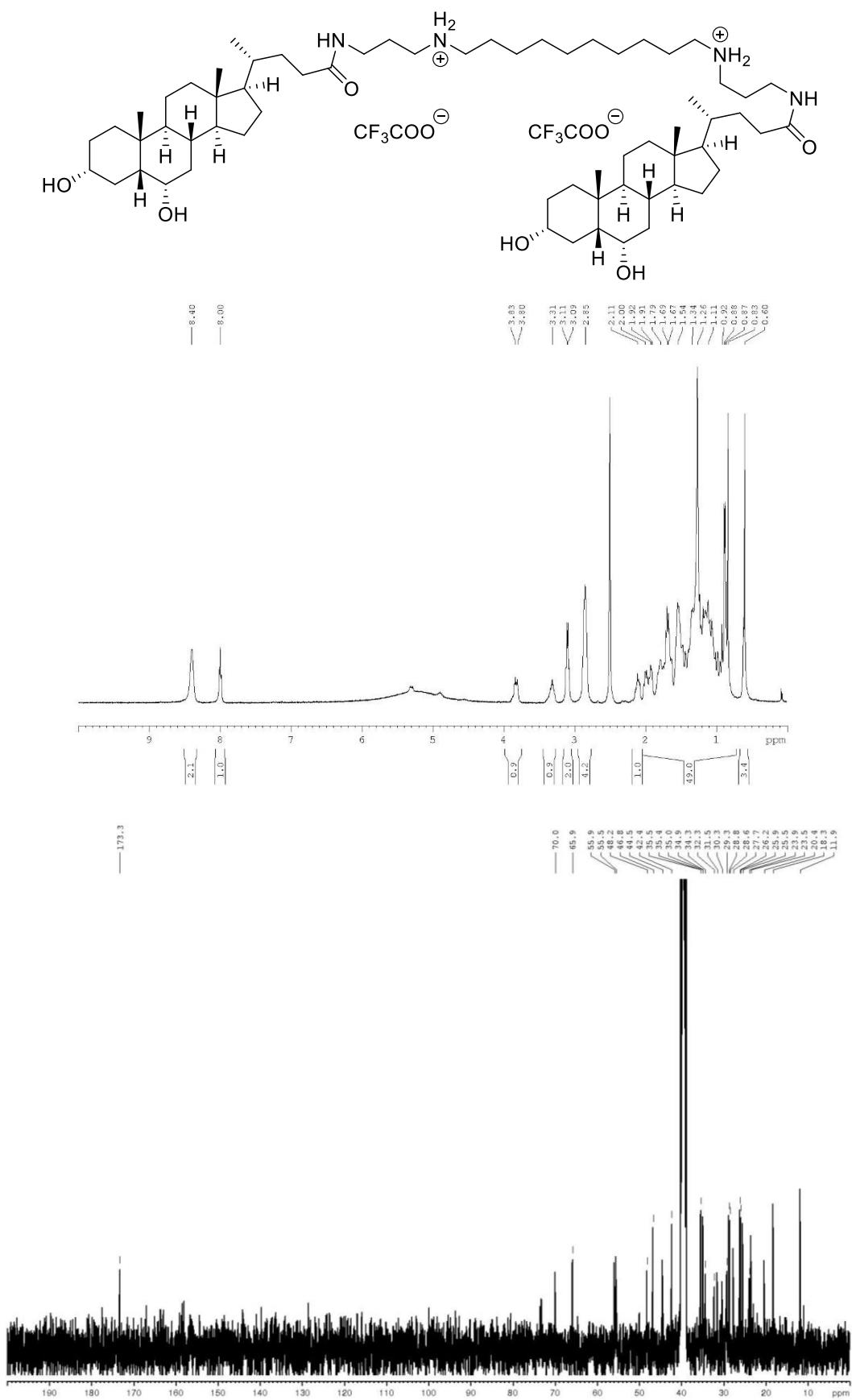


Figure S5 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **7e**.

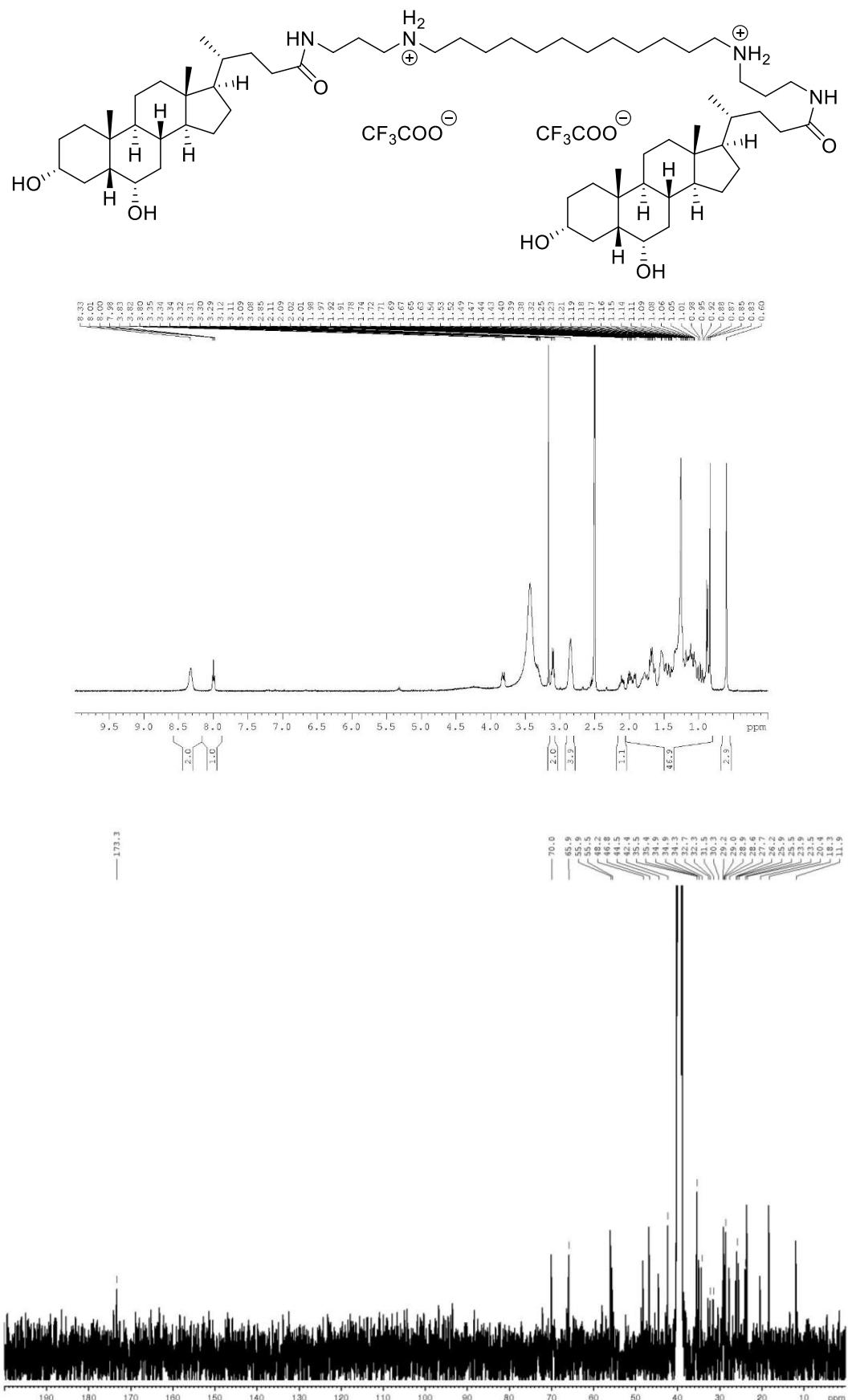


Figure S6 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **7f**.

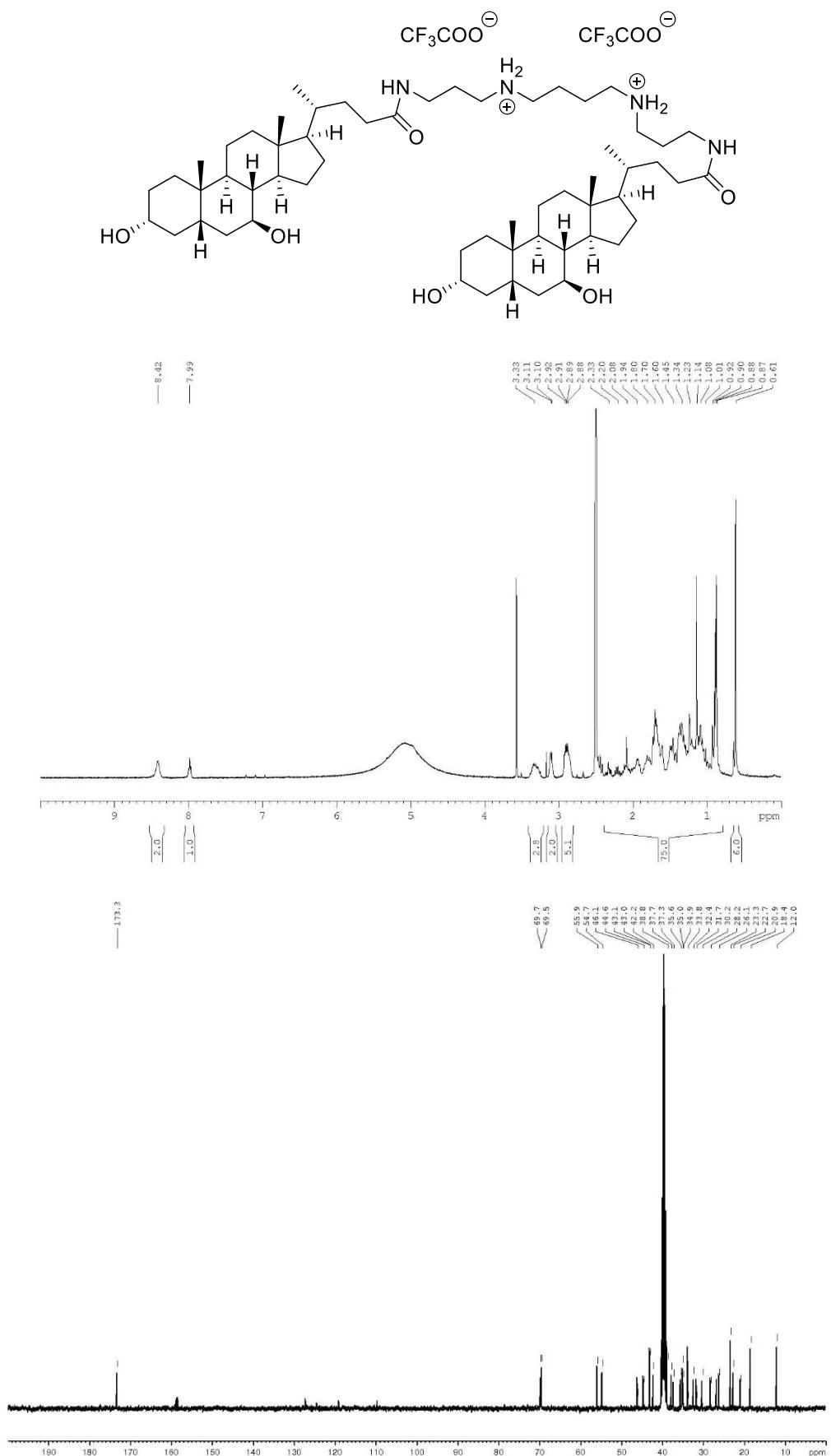


Figure S7 ¹H (DMSO-*d*₆, 400 MHz) and ¹³C (DMSO-*d*₆, 100 MHz) NMR spectra for **8a**.

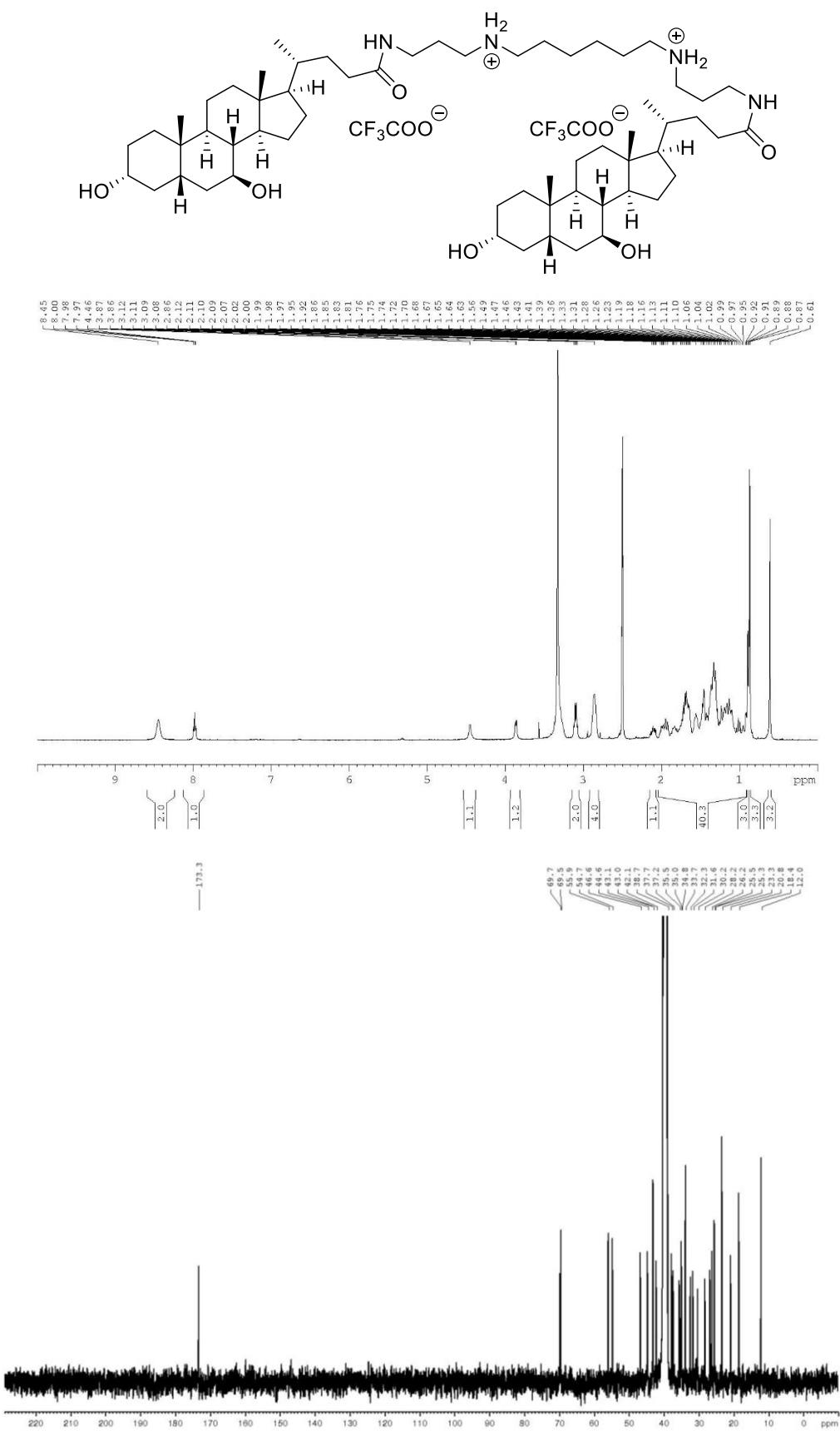


Figure S8 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **8b**.

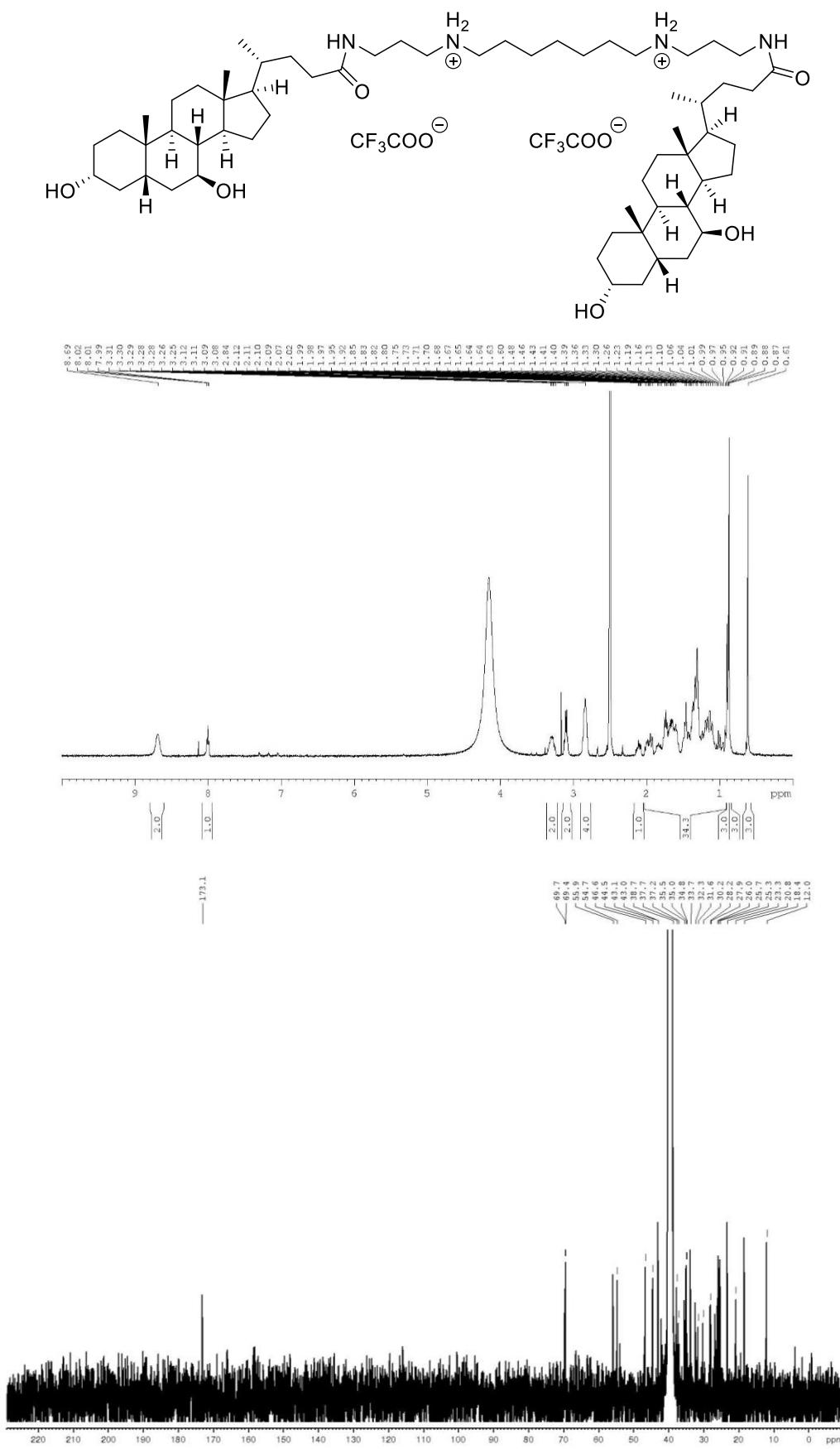


Figure S9 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **8c**.

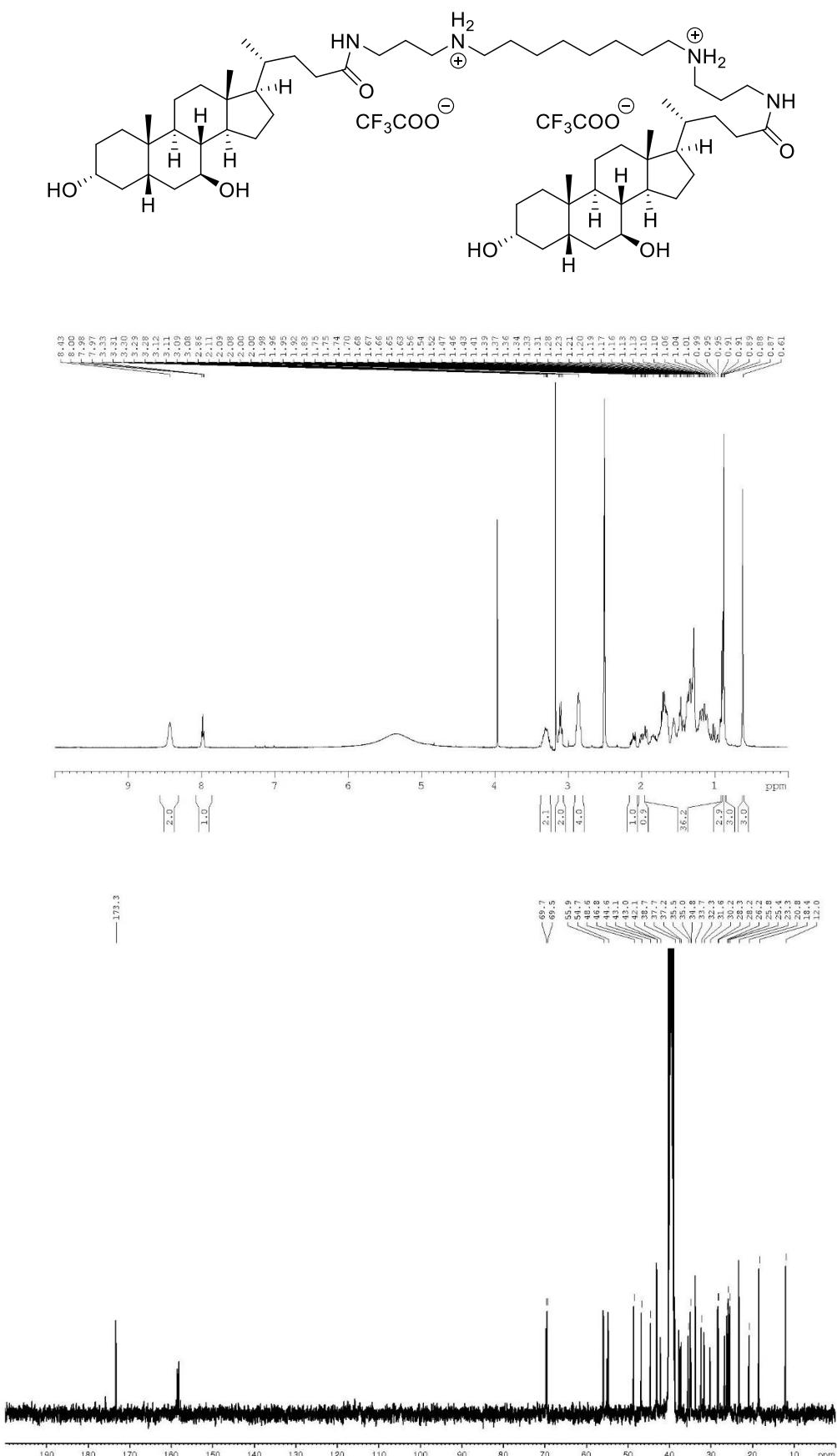


Figure S10 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **8d**.

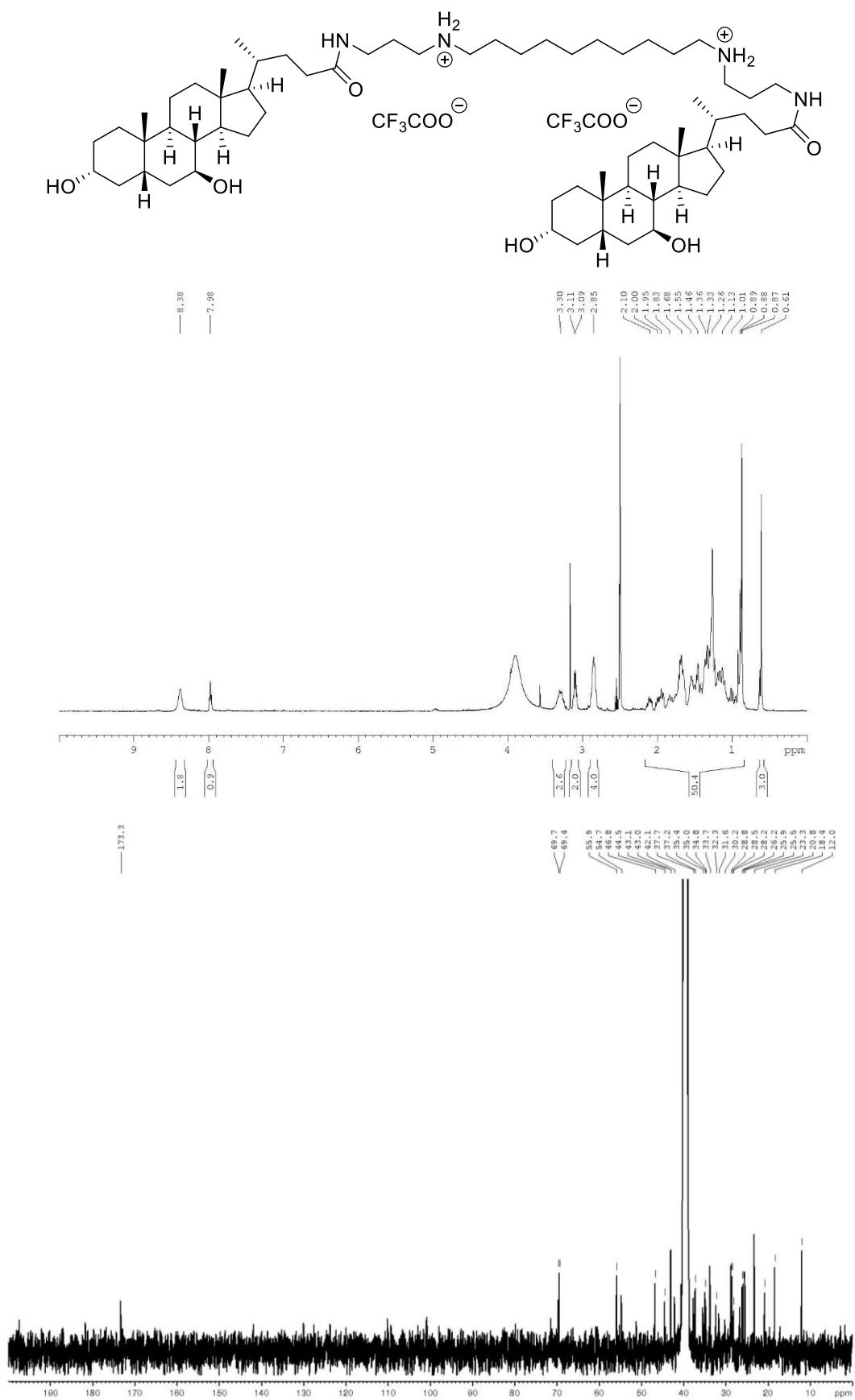


Figure S11 ¹H ($\text{DMSO}-d_6$, 400 MHz) and ¹³C ($\text{DMSO}-d_6$, 100 MHz) NMR spectra for **8e**.

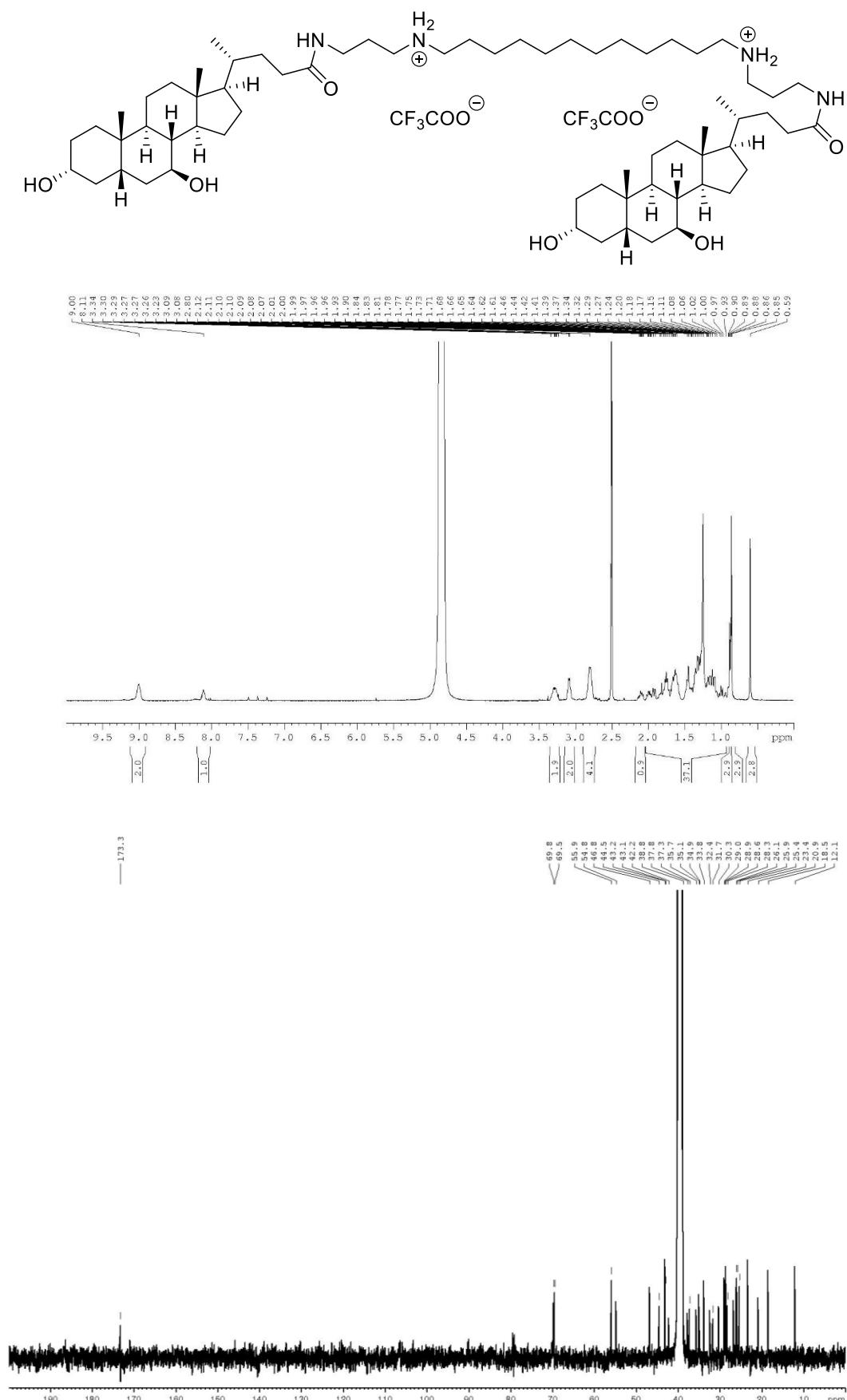


Figure S12 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **8f**.

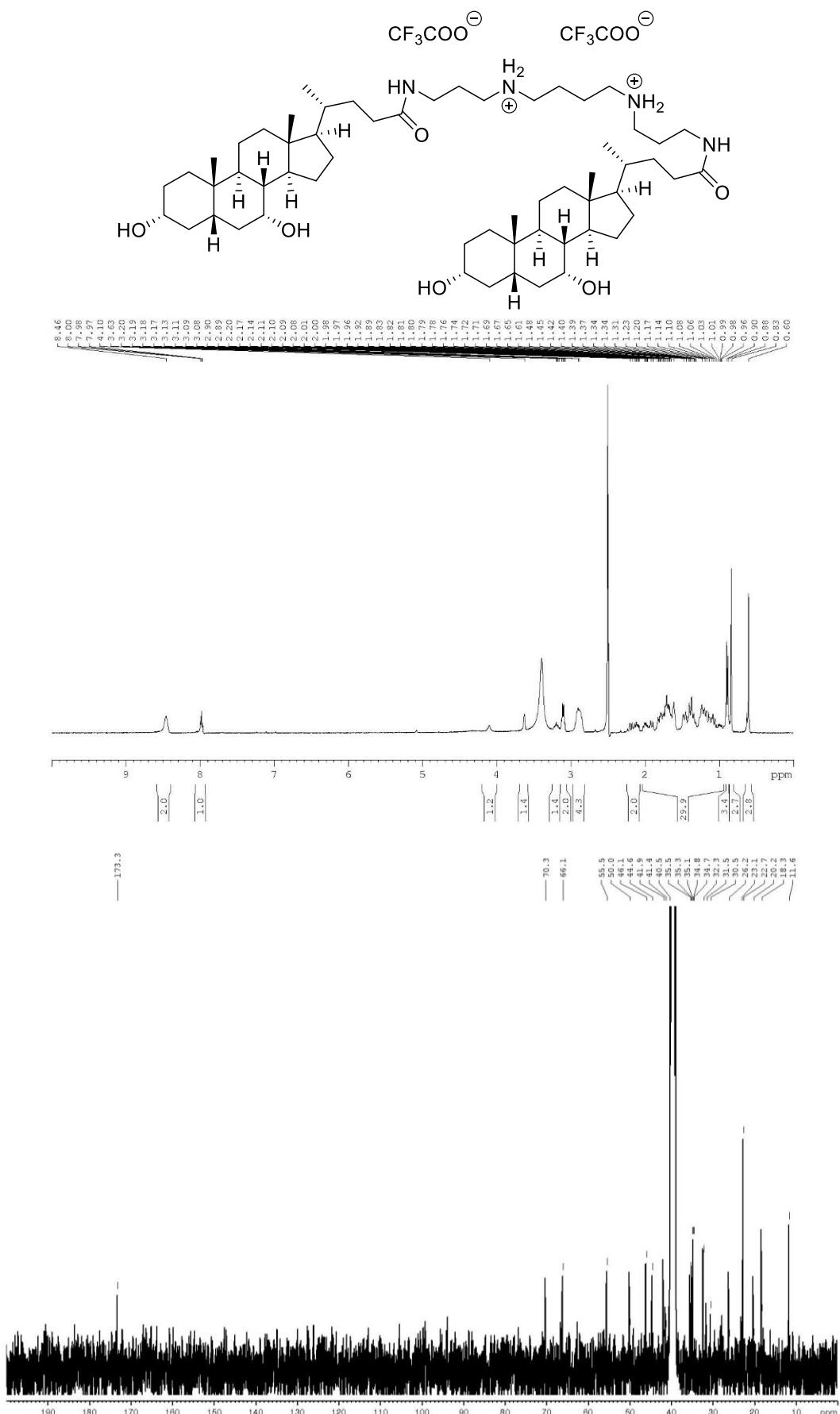


Figure S13 ^1H (DMSO- d_6 , 400 MHz) and ^{13}C (DMSO- d_6 , 100 MHz) NMR spectra for **9a**.