






SUPPORTING INFORMATION

Solubility Enhancement of Mefenamic Acid by Inclusion Complex with β -Cyclodextrin: In Silico Modelling, Formulation, Characterization and In Vitro Studies

Dounia Sid^a , Milad Baitiche^{a,*} , Zineb Elbahri^b, Ferhat Djerboua^a, Mokhtar Boutahala^c , Zouhair Bouaziz^d  and Marc Le Borgne^{d,e*} 

^aLaboratoire de Préparation, Modification et Applications des Matériaux Polymériques Multiphasiques, Département de Génie des Procédés, Faculté de Technologie, Université Ferhat Abbas Sétif-1, Boulevard du Sipion, Sétif 19000, Algérie; ^bLaboratory of Materials and Catalysis, Faculty of Exact Sciences, Djillali Liabès University of Sidi Bel Abbès, 22000 Algeria; ^cLaboratoire de Génie des Procédés Chimiques, Département de Génie des Procédés, Faculté de Technologie, Université Ferhat Abbas Sétif-1, Boulevard du Sipion, Sétif 19000, Algérie; ^dEA 4446 Bioactive Molecules and Medicinal Chemistry, SFR Santé Lyon-Est CNRS UMS3453 - INSERM US7, Université Claude Bernard Lyon 1, Univ Lyon, Lyon, 69373, France; ^eSmall Molecules for Biological Targets Team, Centre de recherche en cancérologie de Lyon, Centre Léon Bérard, CNRS 5286, INSERM 1052, Université Claude Bernard Lyon 1, Univ Lyon, Lyon, 69373, France

* Addresses for correspondence: Milad Baitiche, baitiche_milad@yahoo.fr, Laboratoire de Préparation, Modification et Applications des Matériaux Polymériques Multiphasiques, Département de Génie des Procédés, Faculté de Technologie, Université Ferhat Abbas Sétif-1, Boulevard du Sipion, Sétif 19000, Algérie; Marc Le Borgne, marc.le-borgne@univ-lyon1.fr, Faculté de Pharmacie - ISPB, EA 4446 Bioactive Molecules and Medicinal Chemistry, Université Claude Bernard Lyon 1, 8 avenue Rockefeller, Lyon cedex 8, 69373, France

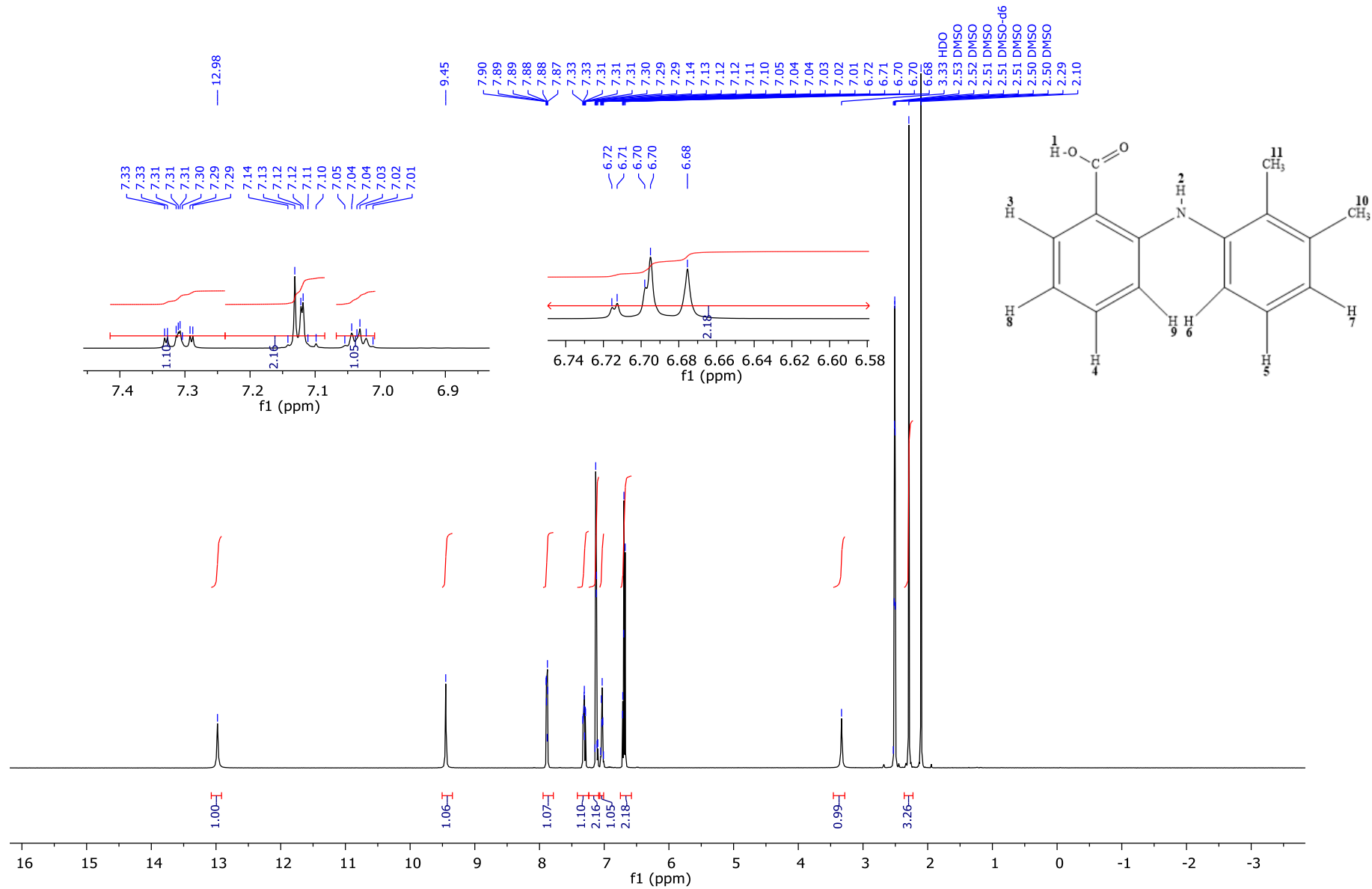


Figure S1. ¹H NMR Spectrum of MA.

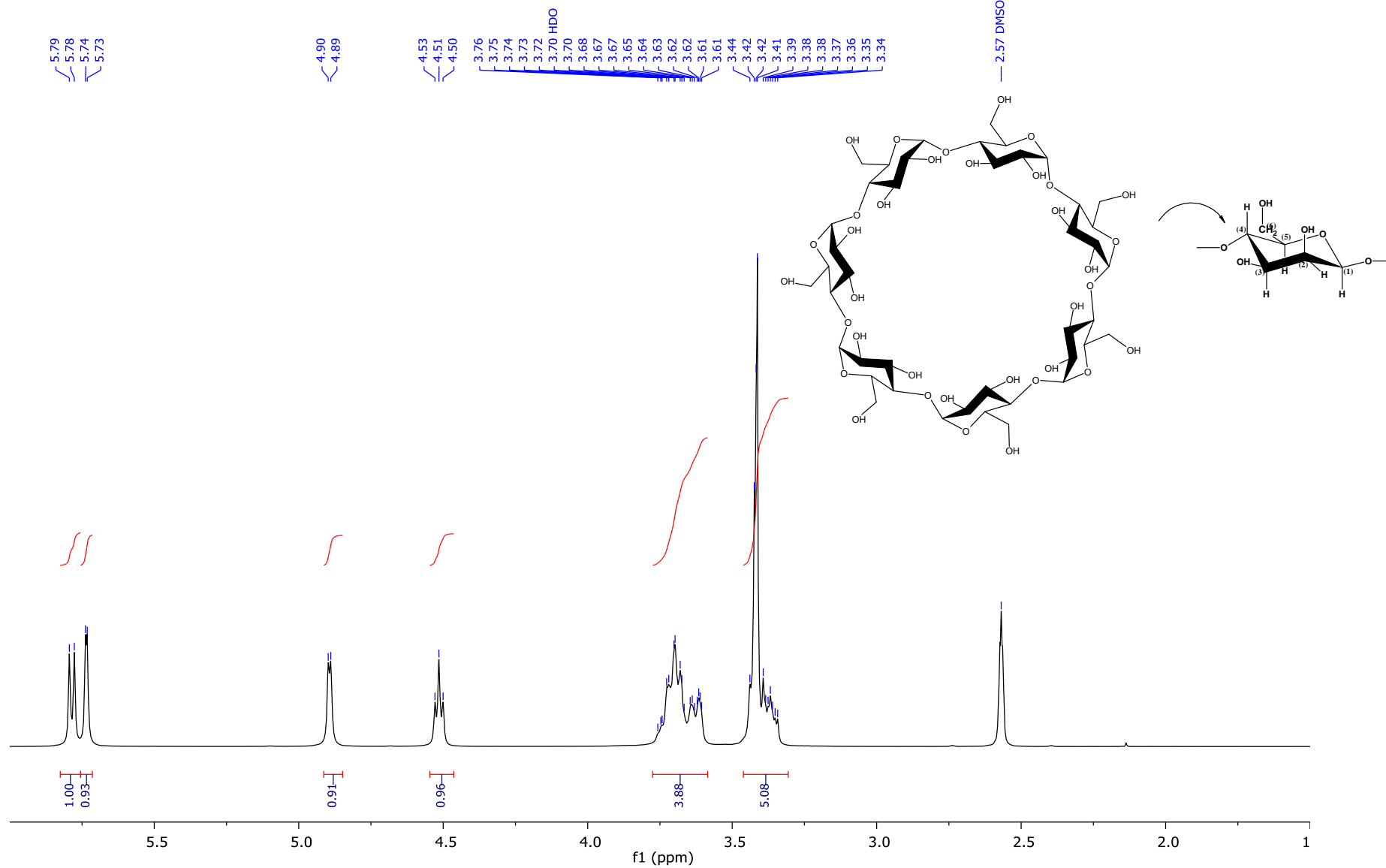


Figure S2. ¹H NMR Spectrum of β-CD.

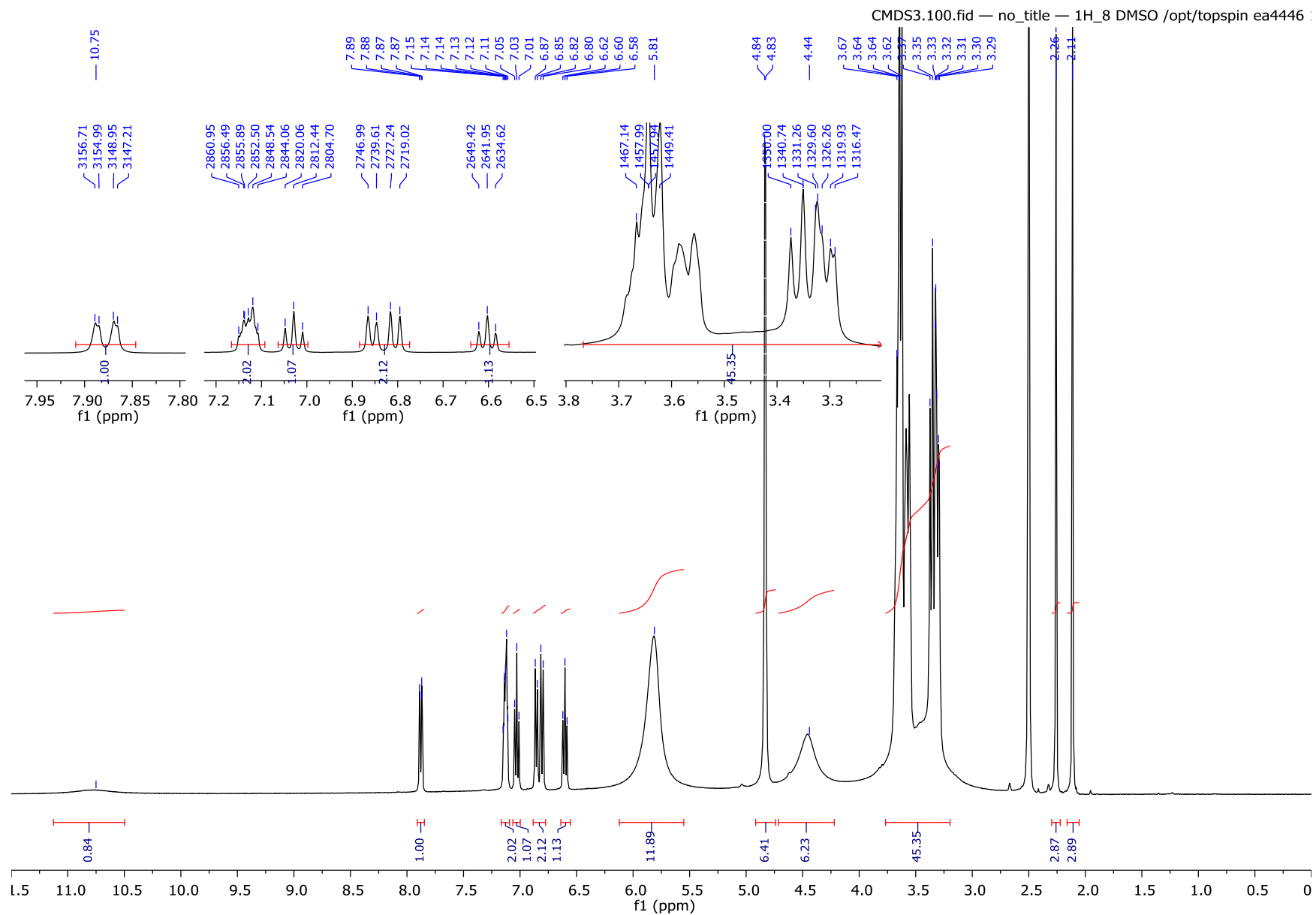


Figure S3. ^1H NMR Spectrum of CE inclusion complex.

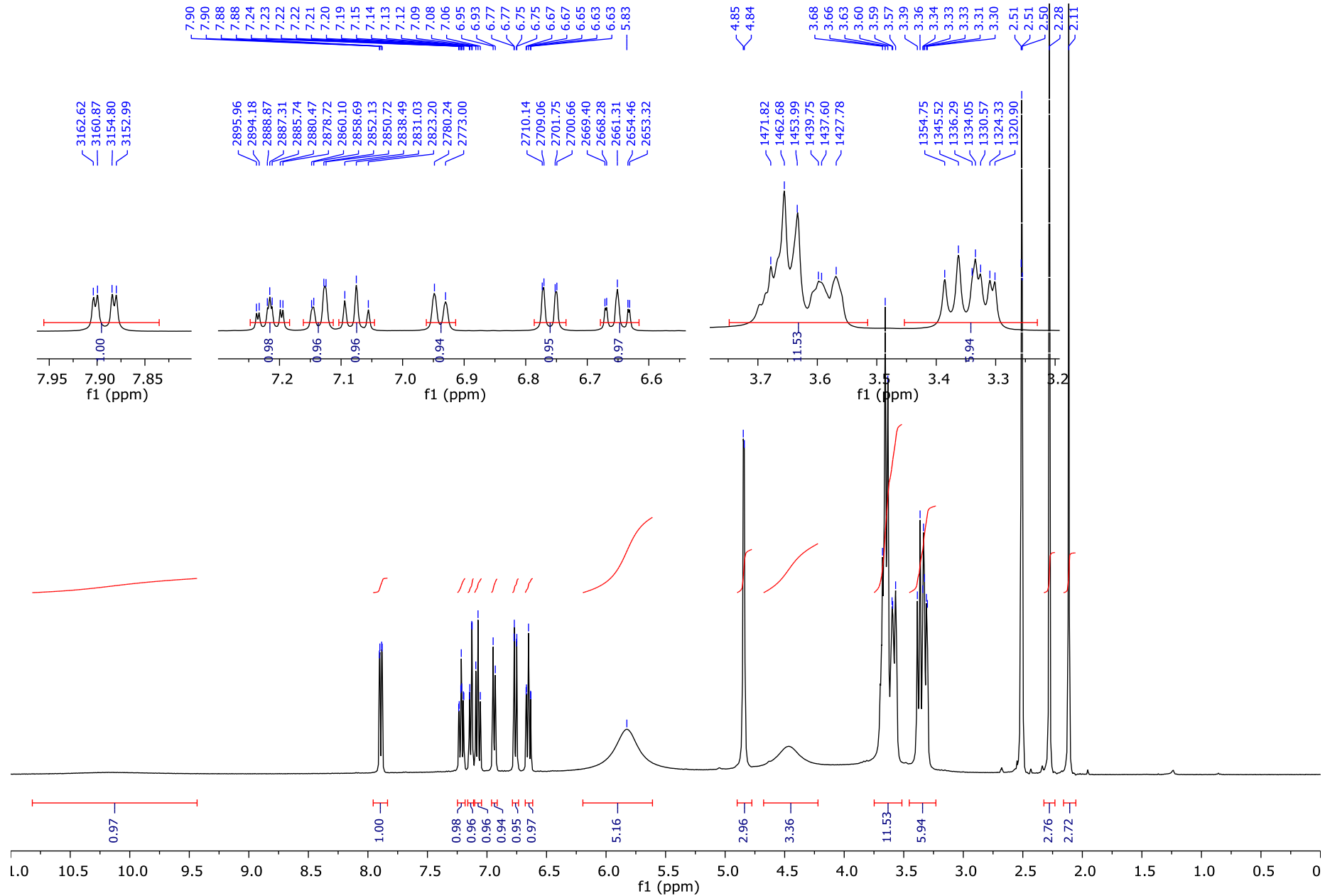


Figure S4. ¹H NMR Spectrum of KN inclusion complex.

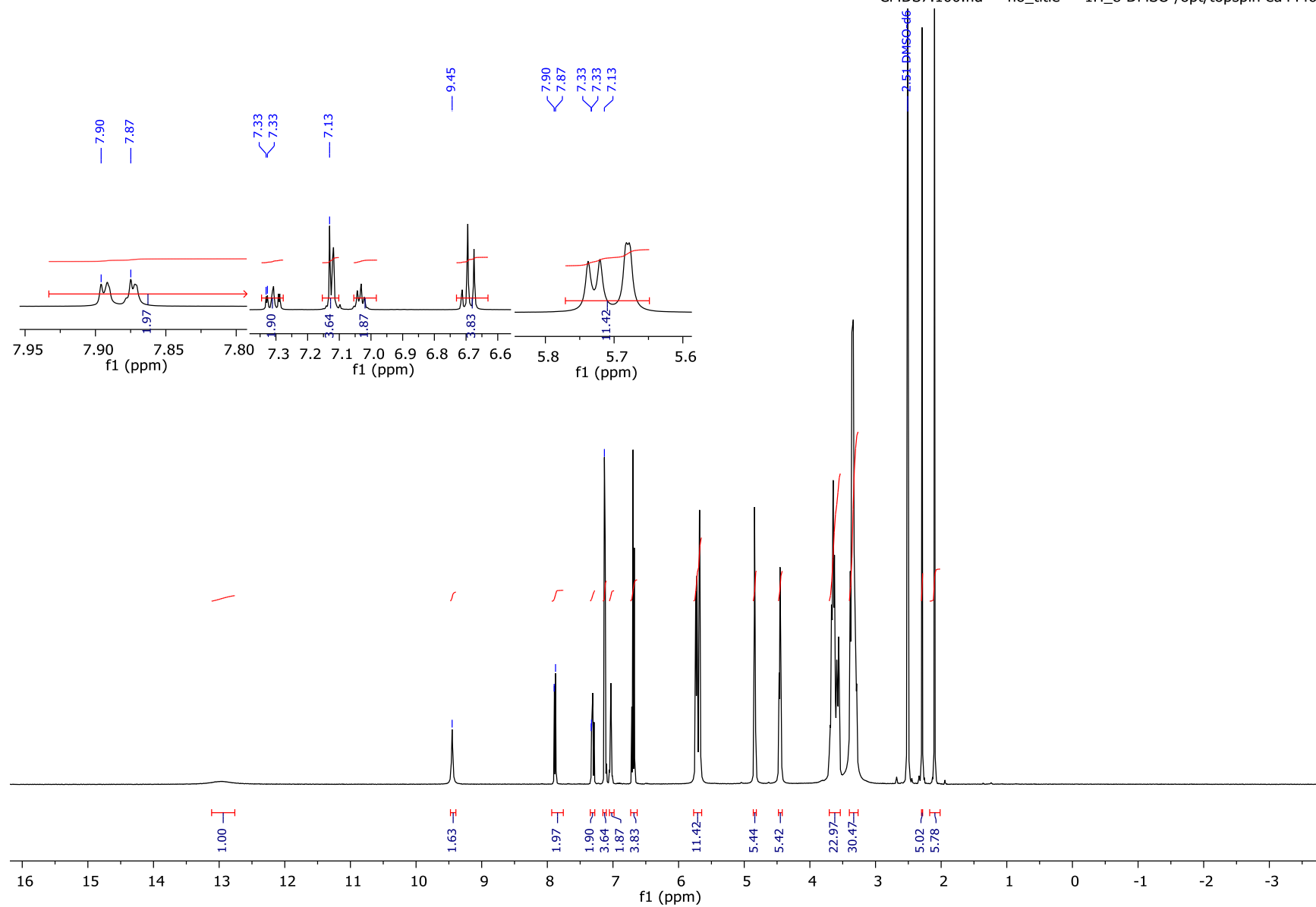


Figure S5. ¹H NMR Spectrum of PM inclusion complex.

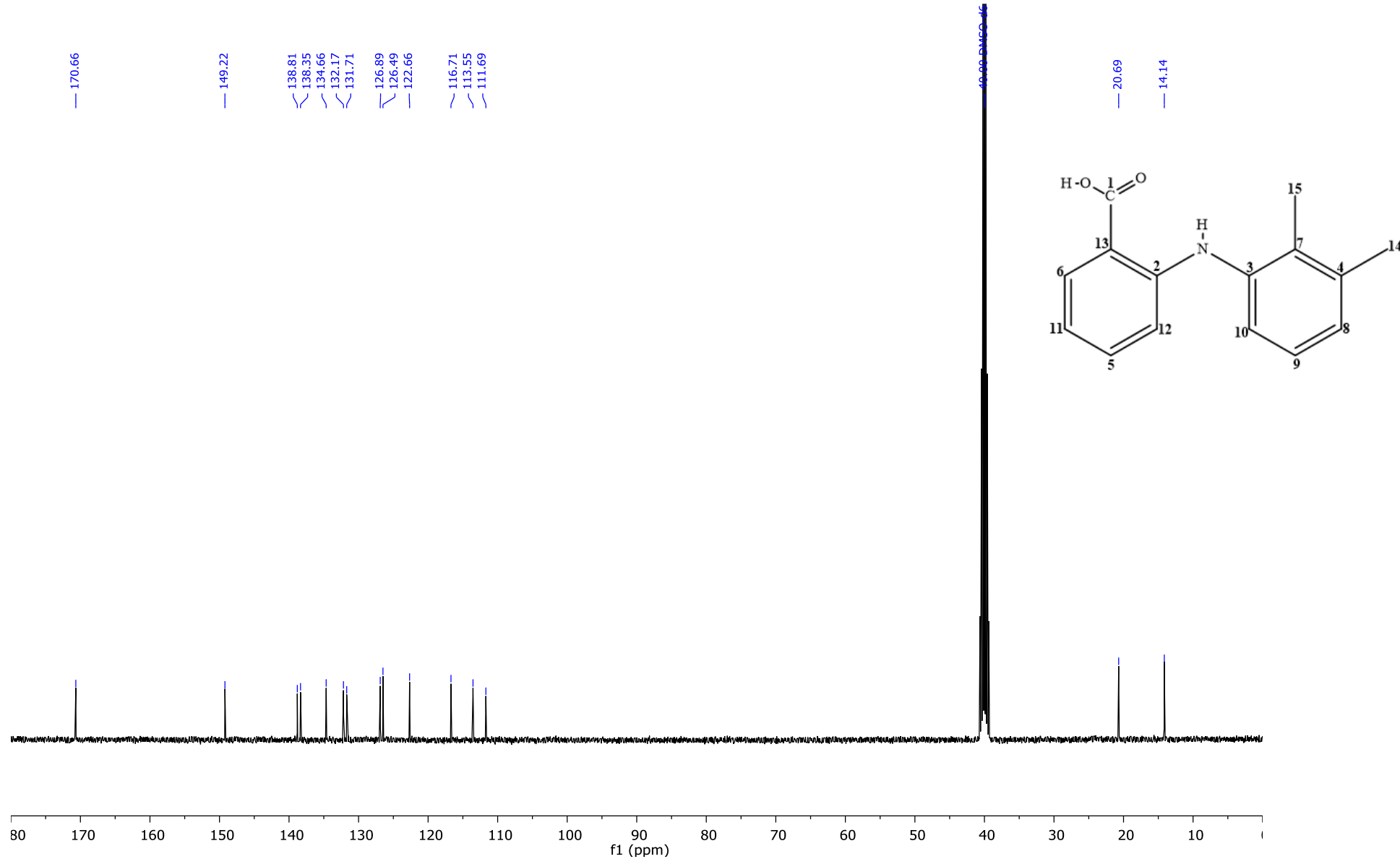


Figure S6. ¹³C NMR Spectrum of MA.

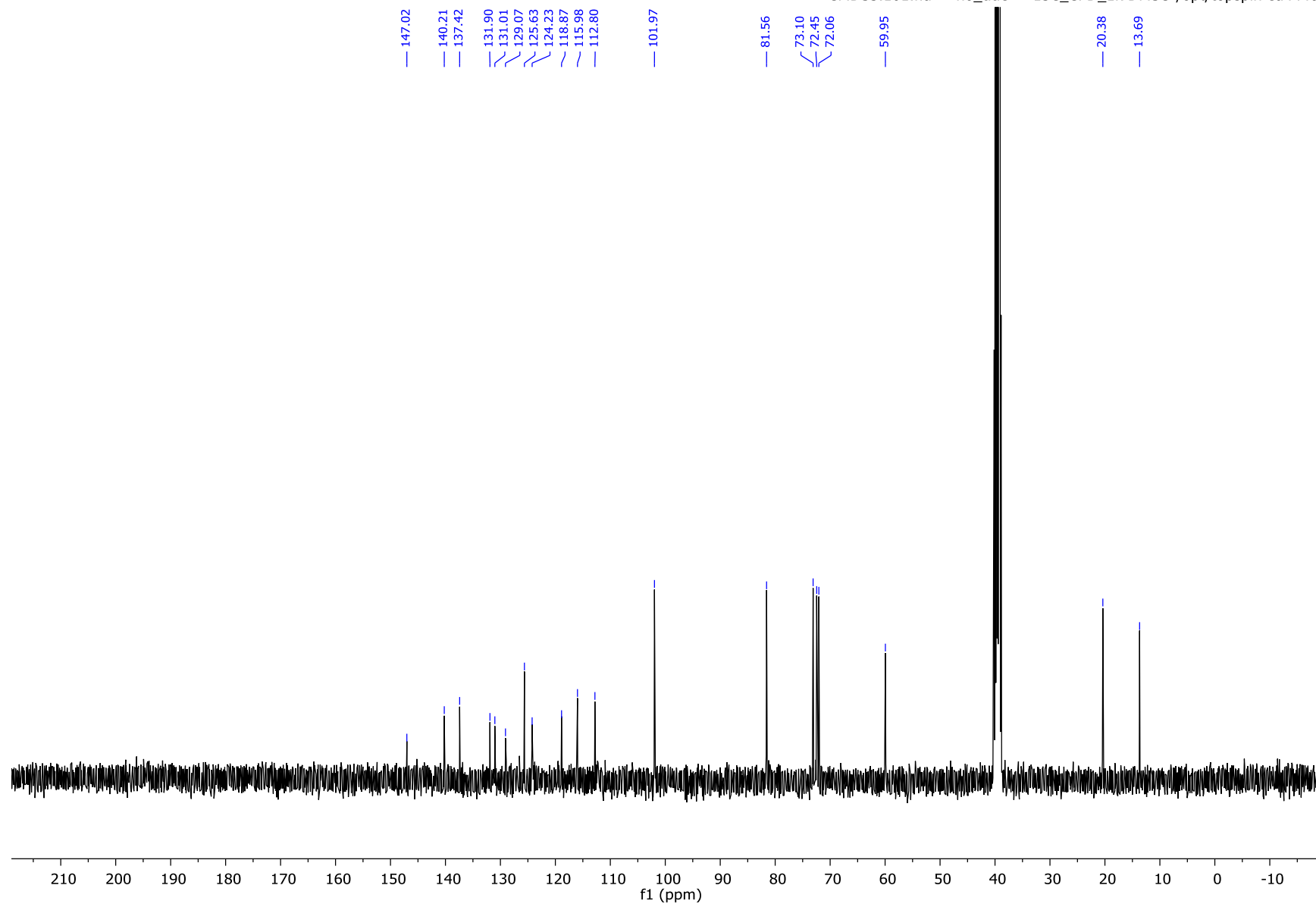


Figure S7. ¹³C NMR Spectrum of CE inclusion complex.

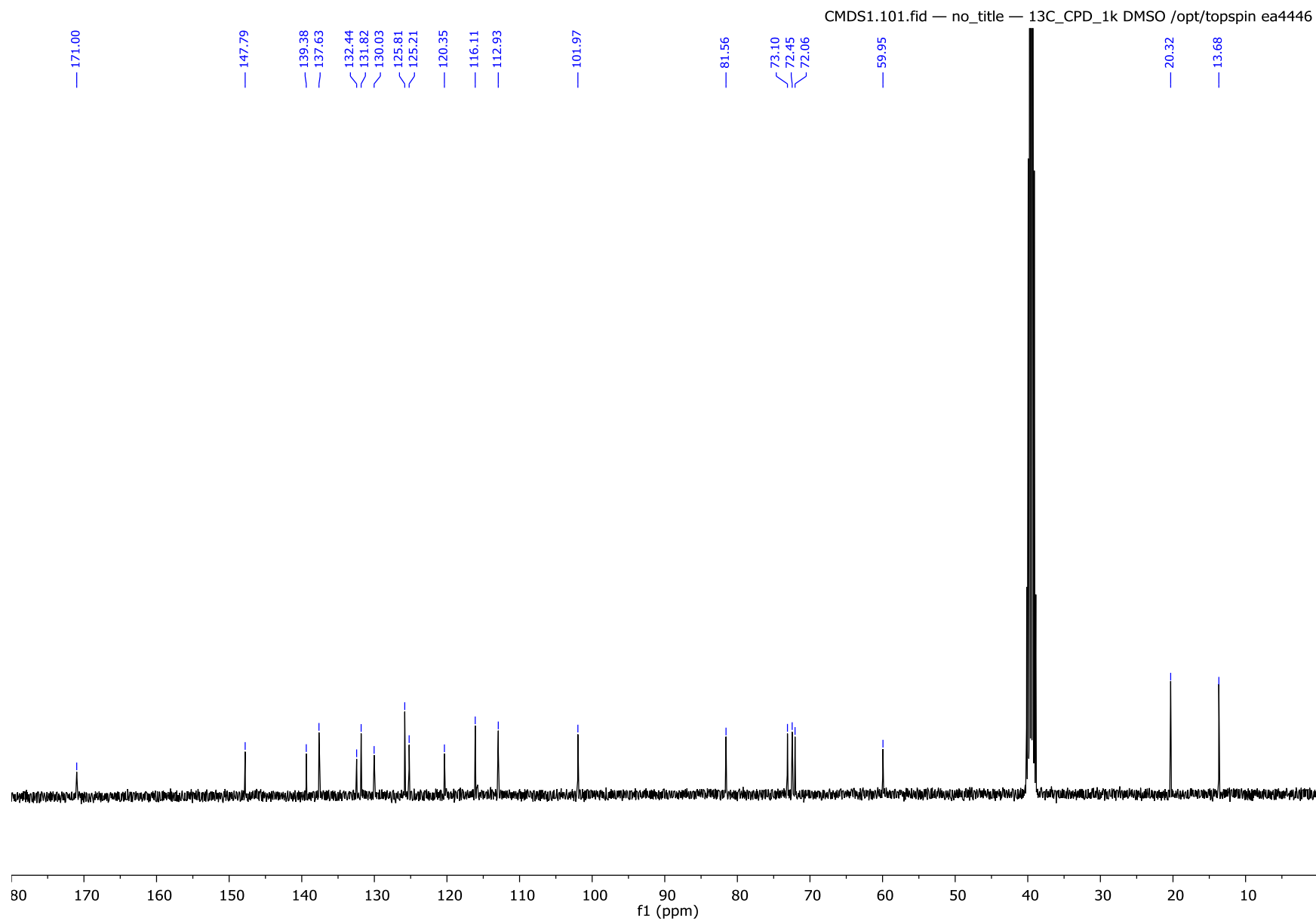


Figure S8. ^{13}C NMR Spectrum of KN inclusion complex.

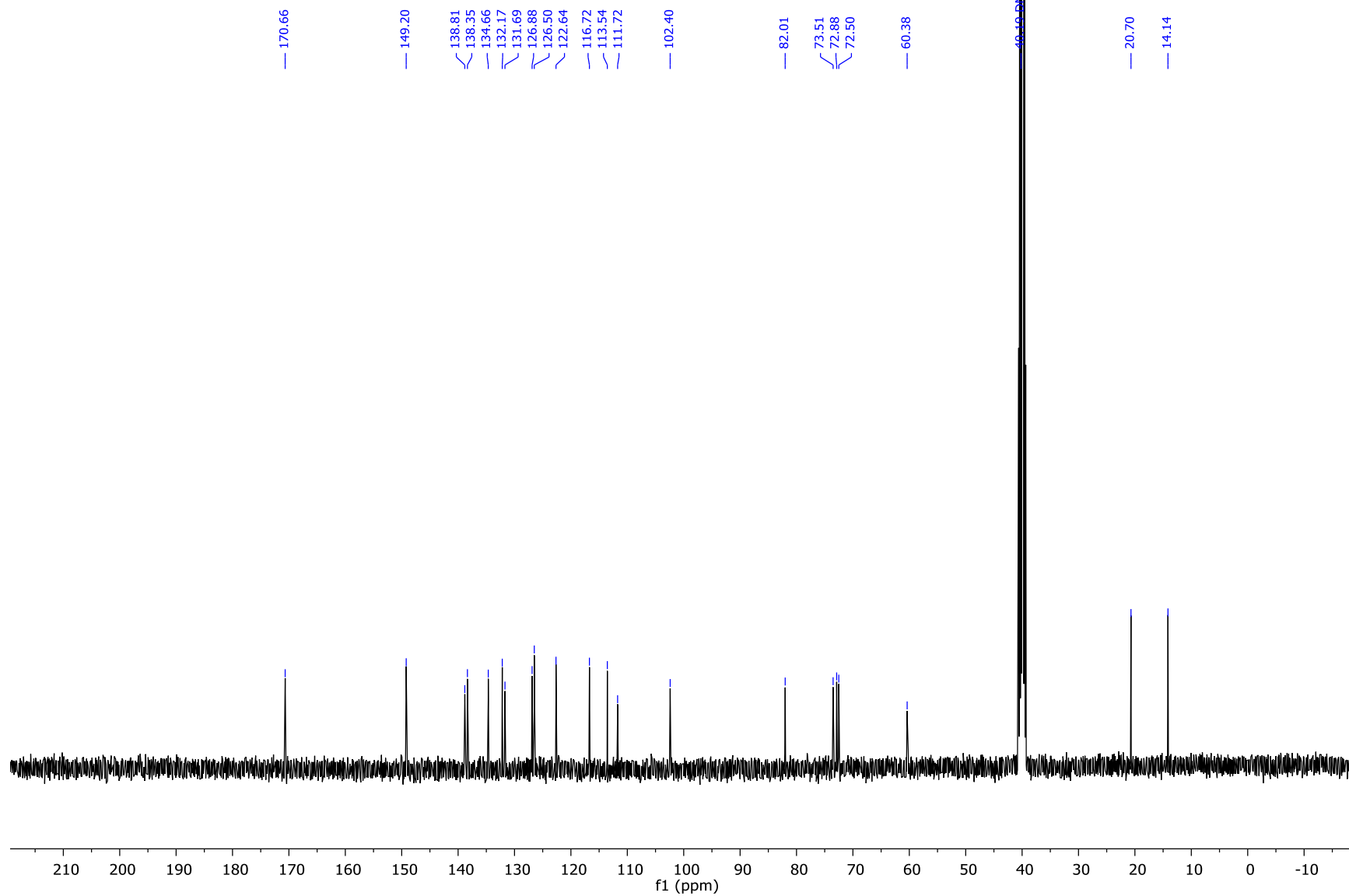


Figure S9. ^{13}C NMR Spectrum of PM inclusion complex.

Table S1. ^1H NMR Chemical shifts (δ , ppm) for CH protons of β -CD alone (δ_{host}) and their complexation induced shifts ($\text{CIS} = \delta_{\text{complex}} - \delta_{\text{host}}$) in $\text{DMSO-}d_6$ at 25 $^\circ\text{C}$.

CH Protons of β -CD	δ_{host}	CIS (CE)	CIS (KN)	CIS (PM)
H-1	4.89	-0.05	-0.05	-0.06
H-6	3.76	-0.05	-0.06	-0.06
H-3	3.70	-0.05	-0.04	-0.05
H-5	3.64	-0.05	-0.04	-0.05
H-4	3.42	-0.06	-0.06	-0.06
H-2	3.37	-0.04	-0.04	-0.04